1	GRUAN OZONESONDE TECHNICAL DOCUMENT
2 3 4	Version 1.1.0.3
5	Purpose of this Guide
6 7 8 9 10 11 12 13 14 15	This Document to GCOS Reference Upper Air Network (GRUAN) ozonesonde operations provides both mandatory operating protocols and non-mandatory recommendations for measurements of vertical ozone profiles using ozonesondes within GRUAN. This Document relies on the standard operating protocols, instrument selection, and uncertainty estimates and calculations from the the WMO/GAW Report #201 [Smit et al., 2014], Assessment of Standard Operating Procedures for Ozone Sondes (ASOPOS) panel recommendations, and the large body of peer-reviewed literature on ozonesondes. This Document also builds on the GRUAN <i>Manual</i> and <i>Guide to Operations</i> (herein referred to as GCOS-171). As in the GRUAN Manual and Guide, mandatory operating protocols are distinguished by the words 'shall' or 'must' while guidelines are distinguished by the words 'could' or 'should'.
16 17 18 19 20 21 22 23 24 25 26	The primary goal of GRUAN is to provide vertical profiles of reference measurements suitable for reliably detecting changes in global and regional climate on decadal time scales. GRUAN's goals have been agreed to by GCOS (Global Climate Observing System) and WMO (World Meteorological Organization). Ozone is classified as a priority 2 essential climate variable (ECV) within GRUAN. GRUAN ozonesonde measurements will provide a calibrated reference standard for global satellite-based measurements of atmospheric ozone. GRUAN ozonesonde measurements will also ensure that potential gaps in satellite measurement programmes do not invalidate the long-term ozone record, and will provide data to fully characterize the properties of the atmospheric column. Because ozone is a key radiatively active gas, vertically resolved measurements of the ozone profile are essential for characterizing radiative transfer through the atmosphere column.
27 28	From Section 6.1 of GCOS-171
29 30 31 32	"GRUAN will not prescribe the use of specific instruments in the network since the emphasis is not on prescribing an instrument, but rather on prescribing the capabilities required of an instrument and allowing individual sites to select an instrument that achieves those capabilities."
33 34 35 36 37 38 39 40 41 42	This GRUAN Ozonesonde Technical Document includes frequent references to the requirements described in the GRUAN <i>Guide to Operations</i> (GCOS-171), and provides additional ozonesonde-specific requirements not described in GCOS-171. It defines the requirements on random and systematic uncertainty and long-term stability for the operations of all ozonesonde instruments in use at GRUAN sites. This Document establishes the philosophy under which GRUAN ozonesondes shall operate and inform current and future GRUAN sites of the expected <i>modus operandi</i> for ozonesonde operations at GRUAN sites. The overall framework under which an ozonesonde will operate in GRUAN is hereafter referred to as the 'GRUAN Ozonesonde Programme'.

- 43 The GRUAN community is not the international authority on ozonesonde operations. This
- 44 Document has been developed in close collaboration with international leaders in the
- development of ozonesonde standard operating procedures (SOPs). These are the principals in
- 46 the WMO ozonesonde community (Dr. H. Smit/Research Centre Jülich GmbH, and collabortors
- 47 who developed ASOPOS), the Network for Detection of Atmospheric Composition Change
- 48 (NDACC) working group, and the principals in the Southern Hemisphere ADditional
- 49 OZonesondes (SHADOZ) network.
- 50 Relevant information from this GRUAN Ozonesonde Technical Document is expected to be
- 51 incorporated into the WMO Manual on the Global Observing System (WMO-No. 544) and the
- 52 Guide on the Global Observing System (WMO-No. 488). This Guide may be additionally
- supported by a series of technical documents listed on the GRUAN web site at
- 54 http://www.gruan.org.

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1 INTRODUCTION

Ozonesonde heritage 1.1.

- 148 Ozone is a key trace gas in Earth's atmosphere. In the stratosphere it absorbs incoming solar
- 149 radiation in the UVC (<280 nm) and UVB (280-320 nm) portions of the spectrum. Because
- 150 radiation at these wavelengths has sufficiently high energy to be detrimental to biological
- 151 systems, the stratospheric ozone layer provides an essential screen thus protect life on Earth's
- surface. During the latter half of the 20th century the stratospheric ozone layer was depleted, most 152
- severely over Antarctica, as a result of anthropogenic emissions of ozone depleting substances. 153
- 154 As a result of the successful implementation of the Vienna Convention for the Protection of the
- 155 Ozone Layer and its Montreal Protocol (including amendments and adjustments to the Protocol),
- 156 emissions of ozone depleting substances have declined dramatically and the status of the ozone
- layer is expected to return to a mid-20th century state in the second half of the 21st century. 157

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159 The effects of ozone are not always positive. Ozone is a key component of photochemical smog 160 and high levels of ozone are associated with poor air quality. The common saving is that ozone is

- 161 'nice from far but far from nice'. Ozone in the troposphere also acts as a strong oxidizer and this
- 162 removes many compounds, including toxic substances, from the air. Ozone levels therefore play
- 163 a role in determining the tropospheric lifetimes of many compounds. Ozone is also a greenhouse
- gas, absorbing outgoing infrared radiation from Earth's atmosphere. Because of its importance 164
- 165 both as an absorber of incoming solar UV radiation, and as an absorber of outgoing infrared
- radiation, it is essential that changes in ozone concentrations throughout the atmosphere are 166
- 167 carefully monitored.

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169 The vertical distribution of ozone in the atmosphere can be monitored using a range of different

- 170 techniques including satellite-based (solar occultation, limb-sounding, nadir viewing)
- 171 instruments, balloon-borne in situ instruments (ozonesondes, dropsondes), and ground-based
- 172 remote sensing systems (lidars and microwave radiometers). Ozonesondes fulfil an important
- 173 role in this suite of techniques by providing very high vertical resolution ozone profiles from the
- 174 surface to the middle stratosphere with small measurement uncertainties, capable of making
- measurements during periods of no sunlight, and can be easily deployed from remote locations 175 176 such as ships or small islands.

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- 178 A number of quasi-independent ozonesonde measurement programmes have been established
- globally to monitor changes in the vertical distribution of ozone. The WMO/GAW¹, SHADOZ 179
- and NDACC communities have established an expert panel. ASOPOS (Assessment of Standard 180
- 181 Operating Procedures for Ozonesondes), to develop standard operating procedures for
- 182 ozonesonde measurement programmes. This Document builds considerably on the large body of
- 183 material already developed by ASOPOS [Smit et al., 2012].

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A complete list of all acronyms appearing in this Document is provided at the end of the document.

- Because long-term satellite-based measurements of ozone in the troposphere and UTLS are not
- currently available, the ozonesonde record provides the primary source for deriving ozone trends
- in the troposphere and UTLS, especially in the climate sensitive region around the tropopause.
- When combined with satellite-based measurements of ozone, they can provide a global, multi-
- decadal data set extending from the surface to the mesosphere for long-term ozone trend
- 190 detection (Bodeker et al., 2012).

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- 192 There are challenges in making ozonesonde measurements such that will meet the needs of
- 193 GRUAN users (see Section 1.2). While instruments may be well calibrated, because instruments
- are seldom recovered after flight, each well calibrated instrument is discarded after each profile
- measurement. Ensuring inter-instrument calibration in an environment where instruments from
- different manufacturing batches may show systematic biases, presents a challenge.

197 1.2. The purpose of ozonesondes within GRUAN

- 198 As detailed in GCOS-112, GRUAN's objectives are to:
- 199 i) Provide long-term high quality climate records;
- 200 ii) Constrain and calibrate data from more spatially-comprehensive global observing systems (including satellites and current radiosonde networks); and
- 202 iii) Fully characterize the properties of the atmospheric column.
- To achieve these goals with respect to ozone, sites within the network should provide vertical
- 204 profiles of reference measurements of ozone for reliably detecting changes in global and regional
- climate, on multi-decadal time scales, for major climatically distinct regions of the globe.
- 206 Changes in ozone, both in the stratosphere and troposphere are known to drive changes in global
- and regional climate. Reference within GRUAN means that, at a minimum, the observations are
- 208 tied to a traceable standard, that the uncertainty on the measurement has been determined, and
- 209 that the entire measurement procedure and set of processing algorithms are properly documented
- and accessible (Immler et al., 2010). Within this framework, ozonesonde measurements are
- 211 classified as ancillary measurements.

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Potential uses of such ancillary measurements include:

- 215 i) Providing measurements at GRUAN sites that complement the priority 1 measurements of temperature, pressure and water vapour and priority 2 measurements of ozone.
- Understanding changes in the vertical distribution of ozone is required to understand changes in the vertical distribution of temperature.
- 219 ii) Providing redundant measurements of the ozone profile.
- 220 The four key user groups of GRUAN ozonesonde ozone profiles are the same as those identified
- 221 in the GRUAN Guide to Operations, viz.:
- 222 i) The climate detection and attribution community. Understanding changes in the vertical
- distribution of ozone is essential to understanding changes in the thermal structure of the
- 224 atmospheric column.

- 225 ii) The satellite community. Validating satellite-based measurements of ozone is recognized as an essential requirement of the GRUAN ozonesonde programme.
- 227 iii) The atmospheric process studies community. High vertical resolution measurements of the
- ozone profile, with well resolved measurement uncertainties, provide key data for
- 229 understanding atmospheric processes. Many aspects of stratospheric dynamics and the
- 230 dynamics associated with stratosphere-troposphere exchange can be studied using ozone
- profiles from ozonesondes. Ozonesonde measurements have played a key role in
- determining ozone loss rates in the Arctic vortex (Rex et al., 1998).
- 233 iv) The numerical weather prediction (NWP) community.

234 1.3. Organization and design of the GRUAN Ozonesonde Programme

- 235 GRUAN operates under the joint governance of GCOS and WMO as a WIGOS Implementation
- 236 Project. A defining attribute of GRUAN is the standardisation and centralization of data
- processing with the goal of ensuring network-wide homogeneity of the resultant data products.

238 *1.3.1.* Terminology

- 239 A GRUAN Ozonesonde Programme is an ozonesonde measurement programme implemented at
- a site and having been assessed and certified as defined in Sections 3.1 and 3.2.
- 241 A GRUAN Ozonesonde instrument is one of the instruments employed in a GRUAN ozonesonde
- 242 programme. These are balloon-borne electrochemical concentration cell (ECC) ozone sensors
- 243 measure high vertical profiles of ozone, pressure, temperature, and relative humidity. ECC ozone
- 244 sensors are described in Section 2.1
- 245 A GRUAN Ozonesonde Product is an ozone product resulting from the measurements made
- 246 within a GRUAN ozonesonde programme. A GRUAN Ozonesonde Product is always produced
- by the GRUAN Ozonesonde Analysis Software System (GOASS, see Section 3.7) designed to
- implement the requirements and recommendations defined in this document.

249 1.3.2. Responsibilities

- 250 The GRUAN Task Team on Sondes (TTS), in consultation with the GRUAN Lead Centre and
- 251 Task Team on Ancillary Measurements, is responsible for integrating best ozonesonde
- 252 measurement practices into GRUAN operations. These best practices shall be synthesized in the
- 253 form of requirements and recommendations compiled in this Document and shall be
- 254 implemented in all certified GRUAN Ozonesonde Programmes.
- 255 GRUAN sites hosting a GRUAN Ozonesonde Programme shall use a designated system of
- 256 methods, techniques and facilities in full compliance with the requirements and
- 257 recommendations detailed in this document. For any given GRUAN Ozonesonde Programme,
- 258 this system will not be changed without advanced notice to the TTS and GRUAN Lead Centre.
- 259 GRUAN Ozonesonde Programmes incorporate a programme to validate the stability and
- 260 uncertainty of the measurements, agreed with WG-GRUAN, and managed in detail by the
- 261 GRUAN TTS and GRUAN Lead Centre. This assurance programme comprises three mandatory
- 262 components, which are the GRUAN Standard Operating Procedures (SOPs) for all GRUAN
- 263 ozonesonde instrument calibration (described in Section 3.5), the RSLaunchClient (described in
- Section 3.6), and the GOASS (described in Section 3.7).

- 265 The design of GRUAN Ozonesonde Programmes shall recognise the heterogeneity of the
- 266 network of sites, many of which will have primary responsibility to networks other than
- 267 GRUAN Ozonesonde Programmes shall integrate, where possible and when feasible,
- with other international long-term monitoring programmes.
- 269 GRUAN Ozonesonde Programmes shall be responsive to the latest technological and scientific
- 270 progress in ozonesonde measurement techniques and observational requirements. Non-GRUAN
- 271 ozonesonde development work can continue at a GRUAN site in collaboration with the TTS
- 272 until mature and validated, at which point any improvements can be introduced into GRUAN
- operations with the agreement of the TTS and GRUAN Lean Centre.
- WG-GRUAN, the GRUAN Lead Centre and TTS will act as the interfaces between GRUAN and
- the community of users of GRUAN ozonesonde products.

276 1.4. Implementation of GRUAN Ozonesonde Programmes

- 277 The implementation of the GRUAN Ozonesonde Programmes, as a whole, and specific issues
- 278 relevant to an individual Ozonesonde Programme shall be guided by the TTS and WG-GRUAN.
- 279 These two teams will work with other relevant expertise in support of GRUAN and coordinate
- with the GRUAN Lead Centre.
- 281 A GRUAN Analysis Team for Network Design and Operations Research (GATNDOR) shall
- 282 undertake focused, short-term research to address specific topics identified by the WG-GRUAN.
- 283 The work will be conducted in coordination with the TTS and with other GCOS programmes
- when appropriate.
- 285 The WG-GRUAN and TTS shall use this report which establishes standard operational
- procedures (SOPs) and metadata requirements for all GRUAN Ozonesonde Programmes. The
- 287 TTS shall evaluate the appropriateness of uncertainty estimates, the usefulness of particular
- 288 measurements and operational procedures, synthesize the available knowledge, and develop
- 289 recommendations to improve GRUAN measurements and operations. The TTS and WG-
- 290 GRUAN shall confer regularly to evaluate the current status of GRUAN observations, to identify
- 291 weaknesses, and to incorporate new scientific understanding into GRUAN. The expertise of
- 292 these teams shall also be used to support the Lead Centre in guiding individual sites through
- 293 changes in instrumentation and operating procedures without impacting long-term measurement
- 294 time series.
- 295 The GRUAN Lead Centre shall identify sites where instrument operators need training, re-
- training, and organise cost-efficient training courses for the network at appropriate locations, as
- 297 advised by the appropriate TTS, to encourage uniformity of instrument operation between sites.
- 298 The Lead Centre may liaise with National Metrological Institutes in this regard.
- 299 All activities associated with the implementation of GRUAN are the responsibility of the
- institution/organization hosting the GRUAN site and should, as far as possible, be met through
- and national funding. To best serve the needs of the climate monitoring and research communities, it
- 302 is essential that GRUAN is cognizant of the evolving science that drives the measurements and
- accuracy of the GRUAN data. The ozonesonde instrumentation deployed and the observing
- schedules may differ between sites, as agreed with WG-GRUAN as part of the site assessment

and certification process, but the methods of observation used with the main observing systems are expected to be uniform between all GRUAN sites.

307 1.5. Links to partner networks and satellite-based measurement programmes

- 309 In the original charter for GRUAN (GCOS-92) it is stated that 'where feasible, the GRUAN sites
- 310 should be co-located and consolidated with other climate monitoring instrumentation'. GRUAN
- 311 Ozonesonde Programmes shall not be run in isolation of existing ozonesonde networks and
- 312 GRUAN is not intended to replace existing networks. GRUAN Ozonesonde Programmes are
- 313 likely to operate in the framework of existing networks such as the Network for the Detection of
- 314 Atmospheric Composition Change (NDACC) and SHADOZ (Southern Hemisphere ADditional
- OZonesondes), and to leverage off the expertise available in these networks and e.g. through the
- 316 GAW (Global Atmosphere Watch²) scientific advisory group for ozone. As a result, close and
- regular coordination between the governing bodies of these networks and with the WG-GRUAN
- and GRUAN TTR+AM is required. This coordination can be achieved by having members of the
- 319 WG-GRUAN and TTR+AM attend steering group meetings of partner networks and by inviting
- 320 co-chairs or steering group members from partner networks to attend WG-GRUAN and GRUAN
- 321 TTR+AM meetings.

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- Where an existing ozonesonde measurement system meets the operational requirements of
- 324 GRUAN, the first priority is to encourage that site to join GRUAN. In such cases operational
- requirements should be optimized to meet the needs of both parties.

326 1.5.1. NDACC (Network for the Detection of Atmospheric Composition Change)

- 327 NDACC comprises more than 70 remote-sensing research sites for observing and understanding
- 328 the physical and chemical state of the stratosphere and upper troposphere and for assessing the
- impact of stratospheric changes on the underlying troposphere and on global climate. A number
- of NDACC sites fly ozonesonde and NDACC has a standing working group on ozonesondes,
- water vapor sondes, and aerosol sondes.

332 1.5.2. GAW (Global Atmosphere Watch)

- 333 GAW is as a coordinated network of observing stations, associated facilities and related
- 334 scientific assessment activities, and supplies basic information to be used by policy-makers
- 335 [Global Atmosphere Watch Guide, GAW Report No.86, 1993]. As a major component of GAW,
- 336 the global network of ozone sounding stations provides the longest time series of the vertical
- ozone distribution between surface and 30-35 km altitude [GAWSIS].
- 338 http://www.empa.ch/gaw/gawsis].

1.5.3. Atmospheric Radiation Measurement (ARM) Programme

- 340 The goal of the U.S. Department of Energy ARM programme is to study changes in climate, land
- productivity, oceans or other water resources, atmospheric chemistry, and ecological systems
- 342 that may alter the capacity of the Earth to sustain life. This includes improving the atmospheric

² http://www.wmo.ch/web/arep/gaw/gaw home.html

- data sets used in regional and global climate models. A primary objective of the ARM user
- 344 facility is to improve scientific understanding of the fundamental physics related to interactions
- between clouds and radiative processes in the atmosphere.
- A dedicated Data Quality (DQ) Office provides ARM with a number of tools to ensure the high
- 347 quality of the collected data. The potential use of these tools in GRUAN must be explored to
- 348 ensure network-wide homogeneity of the GRUAN ozonesonde measurements. The ARM DQ
- Office has developed a suite of sophisticated data quality visualization tools that may be of
- interest to GRUAN Ozonesonde Programmes.

351 1.5.4. SHADOZ (Southern Hemisphere Additional Ozonesondes)

- 352 SHADOZ (Southern Hemisphere Additional Ozonesonde) is a project to augment and archive
- 353 ozonesonde data from over a dozen tropical and sub-tropical sites and has become the central
- 354 repository for vertical profiles of ozone in the tropics/sub-tropics. Prior to the creation of
- 355 SHADOZ, tropical ozonesonde data were accessible via campaigns or collaborative associations
- with specific operating site representatives. Started in 1998 by NASA's Goddard Space Flight
- 357 Center, and other US and international co-investigators, SHADOZ is an important tool for
- 358 equatorial tropospheric ozone research. The rationale for SHADOZ is to: (1) validate and
- improve model and remote sensing techniques for estimating tropical ozone, (2) contribute to
- 360 climatology and trend analyses of tropical ozone and (3) provide research topics to scientists and
- educate students, especially in participating countries [Thompson et al., 2003a; 2003b, 2004,
- 362 2007, 2012]. SHADOZ is envisioned as a data service to the global scientific community by
- providing a central public archive location via the internet: http://croc.gsfc.nasa.gov/shadoz.
- 364 SHADOZ data are mirrored at the Aura Validation Data Center (AVDC) and are deposited to
- WOUDC. While the SHADOZ website maintains a standard data format for the archive, it also
- 366 informs data users of the differing sites' preparation techniques and data treatment. Data from
- 367 launches from various SHADOZ supported field campaigns, such as, the Indian Ocean
- 368 Experiment (INDOEX), Sounding of Ozone and Water in the Equatorial Region (SOWER) and
- 369 Aerosols99 Atlantic Cruise are also available.

370 1.5.5. WOUDC (World Ozone Ultraviolet Data Centre)

- WOUDC operates under the auspices of the WMO/GAW programme to archive ozone and
- 372 ultraviolet in-situ instrument data. Data is contributed to WOUDC at no cost and provides an
- independent storage and backup of instrument data. Like SHADOZ, WOUDC is a web-based.
- public access archive (www.woudc.org) and provides enhanced user search capabilities and
- visualizations. The WOUDC gets guidance from the WMO Science Advisory Groups (SAGs)
- 376 for issues related to both ozone and UV.

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1.5.6. Link to satellite-based measurement programmes

- 379 Ozonesonde measurements have historically provided a key data set for validating satellite-based
- 380 measurements of ozone. GRUAN Ozonesonde Programmes, with their well characterized
- measurement uncertainties and network wide homogeneity are expected to provide a database of
- vertically resolved ozone that will be essential for validating satellite-based measurements of the
- vertical distribution of ozone. Because the GRUAN ozonesonde measurements are likely to
- serve a wide range of end-users within the satellite measurement community, WG-GRUAN and

385 TTR+AM members shall be assigned to liaise with key clients within the satellite community to ensure that GRUAN ozonesonde data products are tailored, where possible, to best meet the 386 needs of this community. Once GRUAN ozonesonde data sets are available, pilot studies on 387 388 enhanced combined data sets using these reference measurements e.g. generating site 389 atmospheric state best estimates (SASBEs) for ozone, need to be undertaken. The GRUAN 390 ozonesonde measurements provide an essential database for removing offsets and drifts between 391 separate satellite-based measurement series within the limitations imposed by the uncertainties 392 on the GRUAN ozonesonde measurements.

2 GRUAN OZONESONDE TECHNIQUES AND MEASUREMENT PRINCIPLES

395 This section provides the GRUAN Ozonesonde Programmes and user community with essential 396 knowledge of the way ozonesondes measure profiles of ozone. For further comprehensive reviews of the ozonesonde measurement technique, the reader should refer to the publications 398 mentioned in this section.

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Ozonesondes are small, lightweight balloon-borne instruments that use an electro-chemical technique to make it situ measurements of ozone from the surface of the Earth to an altitude determined by balloon burst, typically 30 to 35 km [Smit et al., 2002]. The sonde is interfaced to a standard meteorological radiosonde for transmission of the data to the ground and is usually flown together with the radiosonde as part of the same package. The package is carried aloft by a rubber balloon similar to that used for radiosonde measurements, though in this case a 1000-1200 g balloon is typically used rather than the standard 300 g meteorological balloon. The package ascends through the atmosphere at ~6 m.s⁻¹ and, with a measurement frequency of ~2 seconds, results in a vertical resolution of less than 15 m. Ozonesondes constitute the most important data source with long term-data coverage for the derivation of ozone trends with sufficient vertical resolution, particularly in the important, climate sensitive, altitude region around the tropopause.

411 412 413

As defined in GCOS-171:

414 "A reference measurement result typically arises from a defined measurement procedure that 415 involves standards traceable to national or international standards as maintained at National 416 Metrological Institutes (NMIs). For GRUAN, a reference measurement is one where the 417 uncertainty of the calibration and the measurement itself is carefully assessed. This includes the 418 requirement that all known biases have been identified and corrected, and, furthermore, that the 419 uncertainty on these bias corrections has also been determined and reported. An additional 420 requirement for a reference measurement is that the measurement method and associated 421 uncertainties should be accepted by the user community as being appropriate for the 422 application."

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To produce GRUAN ozonesonde reference measurements, mandatory and recommended processing procedures have been established such that the ozonesonde data products derived shall be reproducible at any time in the future. Section 2 describes the data processing procedures required for each component of the ozonesonde measurement technique. The GRUAN Ozonesonde Programmes and centralized ozonesonde data processing facility shall apply these procedures to create the standard reference GRUAN ozonesonde data product (see Sections 3.5 -3.7).

- 432 As of the time of the development of this Technical Document, the Electrochemical
- 433 Concentration Cell (ECC) sonde (Komhyr, 1969) is the only type of ozonesonde being flow and
- therefore this document focusses solely on SOPs for the ECC sonde type. Two other types of 434
- 435 sondes, namely the Brewer-Mast (BM) sonde (Brewer and Milford, 1960) and the Japanese
- manufactured Carbon Iodide (CI) sonde (Kobayashi and Toyama, 1966) are no longer being 436

- flown operationally. In the last decade long-term BM sonde sites have changed to ECC sondes.
- The homogenization of time series that use BM and ECC sondes at the Uccle, Belgium, site has
- been undertaken by De Backer [1999] using results from dual BM/ECC sonde launches [De
- Backer et al., 1998] see also Section 7.2 on the use of transfer functions for homogenizing time
- series that include BM and ECC sondes. Dual flight campaigns at the Payerne, Switzerland, site
- showed no detectable differences between their BM and ECC sondes [Stübi et al., 2008]. Since
- the late 2000s, Japanese sites have switched from using CI sondes to using ECC sondes. While
- Nakamura et al. [2008] conducted inter-comparison studies for CI and ECC sondes, transfer
- functions between the two sensors have not yet been derived.

2.1 The Ozonesonde Measurement

- The ECC instrument consists of a non-reactive teflon gas-sampling pump connected to an ECC
- ozone sensor, and an electronic interface that connects the ozone sensor to a radiosonde for data
- telemetry (see Figure 1 of Komhyr, 1995). The instrument is encased in a polystyrene
- 450 weatherproof box during flight. Measurements of ozone partial pressure, the sonde's pump
- 451 temperature, motor voltage and current, air temperature, air pressure and humidity are
- 452 transmitted to a ground receiving station. Winds derived from GPS-enabled measurements
- became available in the early 2000s.

The ECC sensor measures ozone using iodine/iodide electrode reactions [Vetter, 1967]. Two

- 456 platinum electrodes are immersed in separate cathode and anode chambers, also called half cells,
- of differing concentrations of potassium iodide (KI) solution. The anode cell contains a solution
- 458 saturated with KI. Both cells contain an equal concentration of potassium bromide (KBr) and a
- 459 phosphate buffer to maintain a neutral pH. An ion bridge connecting the two chambers, allows
- ions to flow between the two cells but prevents mixing, thereby preserving their respective concentrations.

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Ambient air containing ozone (O_3) is pumped into the cathode cell and reacts with iodide (I^-) to form iodine (I_2) based on the aqueous reaction:

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$$2KI + O_3 + H_2O \rightarrow I_2 + O_2 + 2KOH$$
 Rxn. 1

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To maintain electrochemical equilibrium iodine is converted back to iodide on the platinum electrode resulting in the release of two electrons by the following reactions:

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In the cathode cell: $3I^- \rightarrow I_3^- + 2e$ Rxn 2

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In the anode cell: $I_2 + 2e \rightarrow 2 I^-$ Rxn. 3

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475 The total cell reaction is the redox reaction: $3I^- + I_2 \rightarrow I_3^- + 2I^-$ Rxn. 4

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Rxn 2 and 3 are rate determining reactions and result in the transfer of ion to the electrode surfaces. An equilibrium exists between I_2 and I_3^- (tri-iodide) when the concentrations of I^- are

479 kept constant.

As a result of the reactions detailed above, each ozone molecule entering the sensor causes two electrons to flow through the ECC's external circuit, which is measured as a current. The resulting electrical current is linearly proportional to the concentrations of ozone in the sampled air. The electrochemical technique assumes no secondary reactions take place and a 1:1 stoichiometric relationship of the I₂:O₃ ratio is maintained. The relationship between ozone and the electrical current (measured in µA) is computed using:

488 Eqn. 1 $P_{O3} = 4.307 \times 10^{-4} (I_{M}-I_{BG})T_{P}\Phi\psi$ 489

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491 where

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493 $P_{O3} = Ozone partial pressure (mPa)$

494 $I_M = Cell current (\mu A)$

495 I_{BG} = Cell background current (μ A)

496 $T_P = Ozonesonde pump temperature (K)$

497 Φ = Pump flow rate (s/100cm⁻³)

498 ψ = Pump flow conversion efficiency (1/pump flow correction factor, unitless)

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The constant, 4.307×10^4 , is the half ratio of the ideal gas constant to Faraday's constant. Measurement techniques and uncertainty estimates for each variable in Eqn. 1 are reviewed below. The cell current, I_M , and pump temperature, T_p , are in situ measurements while the cell background current, I_M , and flow rate, Φ , are measured during pre-flight preparations under ambient laboratory conditions and are assumed to remain constant throughout the flight. While it is preferable that the conversion efficiency, ψ , is determined for each flight, unless automated, this can be very time consuming and as a result ψ values are usually taken from a table of pump flow measurements made at varying low pressures to account for the decrease in pump efficiency at low temperatures. Uncertainties on ψ are expected to be smaller if they are determined individually for each flight rather than taken from a table (which needs to also provide the statistical uncertainty on the ψ values). ψ values vary with ECC sensor type and are further explained in Section 2.5.

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2.2 Measuring the background current

- The background current (I_B) is the residual current measured by the sonde when sampling ozone-
- 516 free air. Conventional processing of the sonde telemetry assumes that the background current
- remains constant during flight and the same assumption is made when processing ozonesonde
- data within GRUAN. As seen in Equation 1, the background current is subtracted from the ECC
- sensor current to infer the ozone partial pressure. In the initial conditioning procedure, both
- 520 cathode and anode cells are filled with sensing solution and stored for no less than 3 days prior to
- launch to reduce the background current and improve the sensor response time (i.e. the time it
- takes for the sensor electronics to respond to a change in ozone concentration) [Kohmyr, 1986;
- 523 1997]. Kohmyr and Harris [1971] show that the background current decreases after the ECC is
- stored for several days while charged with their working solutions; they call this process 'self-
- 525 cleaning'.

GRUAN protocols for measuring background current

GRUAN follows the WMO/GAW SOPs for background current measurement [Smit et al. 2014] requiring three background measurements as detailed below.

- 1. Initial conditioning, i.e. the conditioning procedures when the sensor is first taken out of the box, shall occur no less than 3 days before the ozonesonde flight As this is the minimum acceptable period for the background current to decrease to within the thresholds defined below.
- 2. Day of flight preparations shall be made no more than 7 days after the initial conditioning. If more than 7 days have elapsed, then the cathode and anode chambers must be replaced with fresh solution and initial conditioning procedures must be repeated. Dates of repeated solution change shall be documented in the metadata for collection by the GRUAN RSLaunchClient (addressed in Section 3.6).
- 3. I_{B0} is recorded when the calibration/ozonizer unit is used to run ozone-free air through the sensor, filled with fresh solution, for 10 minutes.
 - a. Following BESOS procedures [Deshler et al, 2008] ozone-free air is run through the sensor until the background no longer drops or until the background current is less than $0.05~\mu A$.
 - b. If the background current does not drop below $0.05~\mu A$ after 20 minutes, the solutions must be changed and the background current measurement repeated. If, after another 20 minutes, the background does not fall below $0.05~\mu A$ the final value should be recorded in the metadata check list, regardless. Ideally, these steps should bring I_{B0} below the $0.05~\mu A$ threshold value.
- 4. I_{B1} is recorded after the response time measurement, i.e. the time required for the sensor current to drop from 4 μ A to 1.5 μ A, and after an additional 10 minutes of ozone-free air has been flushed through the cells. This value may be higher than I_{B0} .
- 5. I_{B2} is recorded prior to launch with the ozonesonde intake tube fitted to an ozone destruction filter. This value may be higher than I_{B0} .

All three background currents shall be recorded by the GRUAN RSLaunchClient (see Section 3.6). Historically, operators have used I_{B2} as the value for I_B in Eqn. 1. In recent years other methods of applying background currents have been employed, such as the minimum of the three background currents [Ryan Stauffer/Penn State, personal communication], a laboratory determined I_B [Holger Vömel/NCAR, personal communication], or I_B set to an upper limit value for those background currents that exceed a maximum threshold based on average I_B measured under optimal laboratory conditions [Bryan Johnson/NOAA, personal communication]. For the GRUAN central processing of ozonesonde flight data, I_{B0} shall be used as the background current for the following reasons:

• The quality of the ozone destruction filter under launch conditions (non-laboratory controlled environment) used to measure I_{B2} cannot be assured to be uniform between flights which introduces a source of random uncertainty which cannot be easily quantified [Reid et al., 1996]. This is particularly the case when ozonesondes are flown in

- the tropics where high humidity affects the ozone removal efficiency of the filter [Newton et al., 2016].
- The use of I_{B2} as the background current is likely an overestimate of the true background current which then leads to an underestimate of the ozone partial pressure. In particular, tropical and polar ozone profiles are strongly influenced by the magnitude of the background current [Reid et al, 1996; Vömel and Diaz, 2010; Newton et al.; 2016].
 Under mid-latitude and tropical conditions, Smit et al. [2014] show that background currents ranging from 0.05 to 0.1 μA contribute 10-20% and 20-40%, respectively, to the measured cell current in the free troposphere.
 - I_{B1} is excluded as an option since it can be biased high. The 10-minute flow of ozone-free air after ozone exposure is arbitrary and likely not representative of the true background current [Thornton and Niazy, 1982; Vömel and Diaz, 2010; Bryan Johnson/NOAA, personal communication]. Laboratory experiments by Vömel and Diaz [2010] identified the decay of the cell current after exposure to ozone and showed that the current does not relax to pre-ozone values after 10 minutes of ozone-free air and that a much longer period of time (hours) is required to approach initial values. The BESOS field campaign [Deshler et al, 2008] found similar enhancements in the background current after ozone exposure. The elevated cell currents indicate a slower decay in the sensor response suggesting that the flushing of ozone-free air for 10 minutes through the cells is not long enough to reduce the cell current to pre-ozone exposure values.
 - A field study conducted by Newton et al. [2016] found stable low background currents when the ozone exposure test during the day of flight preparations was ignored.

Using I_{B0} ensures that background currents are measured under stable, controlled laboratory conditions where uncertainties can be more robustly quantified.

When I_{B0} exceeds 0.05 μA the following steps shall be taken:

- 1. If a solution change, followed by a reasonable length of time running zero ozone air does not bring I_{B0} below 0.05 μ A, then the minimum of I_{B0} , I_{B1} , and I_{B2} shall be used as I_{B} .
- 2. If the minimum background current is still greater than $0.05~\mu A$, then an I_B value of $0.05~\mu A$ must be used. Smit et al. [2012] estimated that properly measured background currents since the mid-1990s should be less than $0.05~\mu A$ in the current generation of ECC sensors. Based on JOSIE results, $0.05~\mu A$ is an upper limit to I_{B0} [Smit et al., 2007].

GRUAN will apply a constant background current correction following WMO/ASOPOS guidelines [Smit et al. 2012; 2014]. Thornton and Niazy [1982] showed that sensors in the early 1980s exhibited negligible sensitivity to O_2 allowing the background current to be treated as a constant. More recent studies support this finding [Smit et al, 1994; Reid et al. 1996; Newton et al., 2016]. Vömel and Diaz, [2010] introduced a modified ozone partial pressure equation that takes into account the excess ozone response due to the buffering of the solution. They measured uncertainties of $0.005~\mu A$ for a 1% full buffer solution and $0.009~\mu A$ for a 0.5% half buffered solution.

Any changes to the treatment of ozonesonde background currents to those described above must be founded on JOSIE-type experiments, followed by rigorous assessment.

2.3 Effects of different sensing solutions and ozonesonde type

While the fundamental chemistry and operating mechanics of the ECC sonde have remained largely unchanged, the KI solution concentrations have varied over the past decades in attempts to improve the measurement accuracy and stability. Inter-comparison campaigns and laboratory studies have been conducted to evaluate the ECC sonde performance using different sensing solution recipes with current sensor types [Hilsenrath et al., 1986; Boyd et al., 1998; Johnson et al., 2002; Smit et al., 2007; Deshler et al, 2008]. The JOSIE studies have shown that the precision and accuracy is strongly dependent on the ozonesonde type and solution [Smit et al., 2007]. JOSIE experiments reveal that differences in instrument construction between SPC and ENSCI significantly impacts the ozonesonde performance.

A variety of sensing solution concentrations and pH buffers are typically used in ECC sondes (see Table 2.3.1) The anode solutions are prepared by saturating the cathode solution with KI crystals.

Table 2.3.1

		pH Buffer, g/L		
Sensing Solution Type	KI, g/L	NaH ₂ PO ₄ •H ₂ O	Na ₂ HPO ₄ •12H2O	
1.0% KI, full buffer	10	1.25	5.0	
0.5% KI, half buffer	5	0.625	2.5	
2.0% KI, no buffer*	20	0	0	
1.0% KI, 1/10 th buffer*	10	0.125	0.5	

^{*} Used at NOAA-led ozonesonde stations only.

The 1.0% KI with full pH-buffer is the conventional cathode sensing solution used for the ozonesonde types SPC-4A, -5A, and -6A [Science Pump Corporation manual, 1996]. Until 1996, ENSCI advocated using the 1.0% solution formula but then switched to recommending a 0.5% KI with half pH-buffer sensing solution formula after 1996 [ENSCI Corporation manual, 1996]. Johnson et al. [2002] introduced the 2.0% non-pH-buffered solution with no KBr that all NOAA-led ozonesonde stations used for a period of almost 10 years in the late-1990s to mid-2000s until switching to a modified 1.0% KI solution using a 1/10th buffer cathode sensing solution recipe. The 2.0% no-buffer solution formula is no longer recommended. The 1.0% KI with 1/10th buffer sensing solution is a relatively new formula and has yet to be included in JOSIE-led evaluation studies. Until that time, only the 0.5% half buffer and 1.0% full buffer sensing solutions shall be used in GRUAN, following WMO/GAW recommendations and as detailed in Table 2.3.2.

Manufacturer/Model	Solution concentration
SPC 6A	1%, full buffer
ENSCI Z, 2Z	0.5%, half buffer

Table 2.3.2 Table of ECC sensors and solution pairing.

The JOSIE-2000 experiment focused on combinations of ECC sensors and sensing solution types to determine the optimal pairing when compared with the world standard UV-photometer.

Results show a reduction in biases for SPC sondes when using the 1.0% KI solution with full buffer pair and for ENSCI sondes that use a 0.5% KI solution with half buffer solution. JOSIE results showed that the SPC/1% and Z/0.5% pairings behave similarly, i.e. measurement differences are within 1.0%.

Homogenizing records that use different sensing solutions

GRUAN recognizes that ECC sensor technology is constantly evolving as solution recipes are fine-tuned to optimize performance and that not all sites coming into GRUAN will operate with the same ECC sensor/solution pairing detailed in Table 2.3.2, e.g. an existing site may continue to use an obsolete sensing solution (e.g. 2% unbuffered) to avoid potentially introducing a discontinuity in the measurement time series, especially if transfer functions have not yet been tested and established.

 Ideally, the ECC sensor and solution type should have a legacy of using one of the two combinations defined in Table 2.3.2. Sites using an ECC sensor/solution type outside of the SPC/1.0% or ENSCI/0.5% pairing should be homogenized with the application of transfer functions (see Section 7.2). Systematic biases between ozone measurements typically result from ECC sensors of the same manufacturing type being operated with different sensing solution concentrations. For ozonesonde sites performing long-term measurements, a change of the sensing solution concentration or ECC-sensor type can introduce a ±5% change, or more, in their ozone records, affecting the determination of ozone trends [Smit et al., 2014].

To support the homogenization of ozonesonde measurement series whose homogeneity is compromised by historical changes in sensing solutions, the ASOPOS working group, as part of the SPARC/IGACO-O3/IOC/NDACC initiative, has established transfer functions based on JOSIE experiments [Smit et al., 2007] for a variety of ECC sensor type and solution strength combinations. Their use allows homogenization of long-term records to conform to either an SPC/1.0% or ENSCI/0.5% sensor/solution pairing (Refer to Section 8.1.2, Table 3 of Smit et al. [O3S-DQA, 2012] for conversion factors). Section 7.2 provides further details and processing protocols involving transfer functions.

While GRUAN Ozonesonde Programmes should commit to using the same ECC sensor and solution type for the lifetime of the measurement programme, changes may be considered if

 Sufficient justification, as determined by the GRUAN Lead Centre and the centralized GRUAN ozonesonde data processing facility, is provided for the proposed change. A balance must be found between GRUAN Ozonesonde Programmes being responsive to the latest technological and scientific progress in ozonesonde measurement techniques and observational requirements, and the importance of avoiding discontinuities in the climate data record.

A new model is developed or a new manufacturer enters the ECC market that recommends a new sensing solution recipe.

Changes in ozonesonde working solutions must be managed through an appropriate change management programme whereby the necessary tests, laboratory studies, and dual sonde launch

campaigns are conducted to characterize any systematic biases, and their uncertainties, in the stoichiometry and response times at all pressure altitudes (see Section 6 on the uncertainty budget). Sites undergoing such change management shall also participate in developing transfer functions required to maintain the homogeneity in the data record.

Ozonesonde expertise outside of GRUAN shall also be used to support the Lead Centre in guiding individual sites through changes in instrumentation without impacting long-term measurement time series.

2.4 Measuring pump flow rate

A common procedure in the ECC conditioning is to use the soap bubble flowmeter method to measure the volumetric flow rate of the pump, Φ [sec/100ml]. The required equipment and set-up are described in the ENSCI and SPC manuals [DMT manual, Appendix D, 2014; SPC manual Section 3.2.1, 1999]. While the ECC is charged with solution and the air pump is operating, the cathode outtake tube is connected to the flowmeter. The air flowing from the ECC pump into the burette allows soap bubbles to rise up the burette. As a single soap bubble rises, a handheld stopwatch is used to determine the time to displace that soap bubble 100 ml. Several flow rates are calculated and the mean is assigned as the final Φ applied in Equation 1. The uncertainty of

The GRUAN procedure for determining pump flow rate is as follows:

the flow rate is small, generally within $\pm 1\%$ [Smit et al., 2014].

1. The flowmeter equipment provided by ENSCI and SPC is standard and reasonably identical. GRUAN will accept either.

2. GRUAN acknowledges that the soap bubble solution recipe varies among manuals and operators and requires only that the same recipe is used throughout the lifetime of the measurement record.

3. The measurement of the flow rate shall be made five times as required by WMO/GAW and implemented in most SOPs.

i. Flow rates that differ by 2 sec/100ml or more from the median after measuring the

flow rate five times should be redone.
ii. Mean Φ should be between 26 and 32 sec/100ml.

 • Lower and upper limits are chosen by consulting pump flow rate ranges found in the SPC manual [1999] and Smit et al., [2014].

 • If the mean Φ is not within the acceptable range, this must be reflected in a the setting of an appropriate data QA/QC flag.

4. As recommended by WMO/GAW, flow rates must be measured on the day of the flight.

Lab temperature, relative humidity, and pressure should be recorded at the time the flow rate measurements are taken to correct for the evaporation of the soap bubble solution (see
 Komhyr et al. [1995], Johnson et al. [2002], and Smit et al., [2014] and Section 8.4).

GRUAN Ozonesonde Programmes must use equation 17 from Smit et al. [2012] to calculate the pump flow rate correction factor, C_{PH}. WMO/GAW defines C_{PH} as

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747 Eqn 2.4.1
$$C_{PH} = \left[1 - \frac{RH_{Lab}}{100}\right] \bullet \frac{P_{H2O,Sat}(T_{Lab})}{P_{Lab}}$$

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where, $P_{H2O,Sat}$ is the saturation vapor pressure under laboratory conditions, i.e. P_{Lab} , T_{Lab} , and RH_{Lab}. C_{PH} is applied to the mean Φ with the expectation that this has a negligible impact on the uncertainty calculations.

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6. The pump flow rate must also be corrected for the temperature difference between the internal pump base temperature and the ambient room temperature. C_{PL} is defined as

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756 Eqn 2.4.2
$$C_{PL} = \frac{T_P - T_{Lab}}{T_{Lab}}$$

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WMO/GAW reports (T_P-T_{Lab}) are on the order of +2K with an uncertainty of ±0.5K.

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760 7. The corrected pump flow rate is then expressed as:

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762 Eqn 2.4.3
$$\Phi_{Final} = [1 + C_{PL} - C_{PH}] \bullet \Phi$$

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Section 6.3 addresses the flow rate uncertainty and its contribution to the ozone measurement uncertainty.

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2.5 Estimating degradation in pump efficiency

- 768 It has been well documented that the efficiency of the ECC pump decreases at high altitudes
- 769 [Komhyr, 1967; 1969; 1986; et al. 1995; Johnson et al., 2002; Smit et al., 2014]. Johnson et al.
- 770 [2002], and references therein, cite pump leakage, dead volume in the piston pump, and back-
- pressure exerted on the pump by the cell solution as main causes of pump efficiency loss at low
- 772 pressures. Experiments reveal that the pump flow rate, Φ , measured at the ground is constant up
- to 100 hPa and decreases steadily to the top of the atmosphere. This is true for the pumps used in
- both SPC and ENSCI ozonesondes.

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- Calculated ozone partial pressures must therefore include a correction for the effects of pump
- efficiency loss. From Equation 1 (in Section 2.1), the pump flow conversion efficiency, Ψ
- 778 (1/pump correction factor), takes into account the efficiency loss in Φ as a function of pressure. 779 Empirical averages obtained from various lab techniques have yielded pump correction factors
- 780 (PCFs; Komhyr [1986]; Komhyr et al. [1995]). The two most widely used PCFs are shown in
- 781 Table 2.5.1. Table 2.5.1 PCFs have been calculated based on SPC ECC type and models older
- than SPC 6A. The sample sizes are small (e.g. K95 N = 13) and it is recommended that
- 783 laboratory studies be conducted to obtain much larger sample sizes of the various ECC models
- currently in use to verify or update the pump efficiency corrections and their uncertainties.

Pressure	Komhyr, 1986	K86 uncertainty,	Komhyr et al.,	K95 uncertainty,
[hPa]	(K86)	ΔΨ	1995 (K95)	ΔΨ
Sfc-100	1.000	1.000	1.000	1.000
100	1.007	± 0.005	1.007	± 0.005
50	1.018	± 0.006	1.018	± 0.005
30	1.022	± 0.008	1.029	± 0.008
20	1.032	± 0.009	1.041	± 0.012
10	1.055	± 0.010	1.066	± 0.023
7	1.070	± 0.012	1.087	± 0.024
5	1.092	± 0.014	1.124	± 0.025
3	1.124	± 0.025	1.241	± 0.043

Table 2.5.1 Pump corrections factors (PCF) with 1-sigma uncertainties. PCF values are taken from the GAW Report No. 201, Table 3-3 [Smit et al., 2014].

Following the recommendations of WMO/GAW report 201 [Smit et al., 2014], GRUAN Ozonesonde programmes shall use the K86 PCFs for SPC ozonesondes and K95 PCFs for ENSCI ozonesondes as listed in Table 2.5.1. PCFs between tabulated values must be interpolated on a log pressure scale with 2nd order polynomial interpolation. Ideally GRUAN should use PCFs derived individually for each sonde. As briefly mentioned above, obtaining PCFs for each sonde should result in smaller uncertainties on PCFs over using tabulated values which represent mean values across multiple samples. However, these measurements are time consuming, require additional hardware and, if made in a non-standard way, could introduce inhomogeneities across the network. See e.g. Figure 7 from Johnson et al. [2002] that shows a significant spread of PCF values that are based on different measurement techniques and different ECC types and models. Methods for calculating PCFs are not standardized in the ENSCI and SPC manuals, nor considered in the WMO/ASOPOS recommendations. While it would be best practice for GRUAN to use PCFs specific to current models, i.e. SPC 6A or ENSCI Z ECC, based on statistically appropriate sample sizes, the resultant look-up tables do not currently exist. GRUAN therefore encourages peer-reviewed laboratory studies that will produce PCFs, with associated uncertainties, specific to manufacturer type and model. Until such results become available, GRUAN shall use the WMO/GAW recommended values tabulated above.

2.6 Measuring pump temperature

The temperature of the ozonesonde pump, T_p, is required in the calculation of the ozone partial pressure (see Equation 1., Section 2.1) to account for the temperature of the air flowing through the pump. Over time, the location of the thermister used to measure the pump temperature has changed, potentially introducing inhomogenieties into the sounding record [Smit et al., 2014]. Smit et al. [2014] has identified five configurations of T_p measurements based on the placement of the thermister (see Table 2.6.1) and has characterized their uncertainty relative to the current placement of thermisters in modern ECC sondes which is inside the pump and is referred to as the internal pump temperature (see Case 5 in Table 2.6.1).

819 Table 2.6.1

Case	Time Period	Location	Name	Sonde Types	Notes
1	1960- end 1980s	Bottom of circuit board	Box Temperature	SPC 2A, 3A, 4A	Analog sondes
2	1990s	Suspended in the styrofoam box in the vicinity of the pump	Box Temperature	SPC 5A	Start of digital sounding systems. Behaves as in Case 3
3	1990s	Taped thermister at the pump base	External Pump Temperature	SPC 5A	
4	1990s	Epoxied at the pump base	External Pump Temperature	SPC 5A	Behaves like Case 1
5	> 1995	Mounted inside the pump body, close to the piston	Internal Pump Temperature	ENSCI Z & 2Z, SPC 6A	Current generation ECC soundings

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Smit et al. [2014] considers the correct or 'true' T_p as the pump temperature measured in the vicinity of the moving piston, T_{piston}. Based on Komhyr and Harris [1971] and JOSIE 2000 lab experiments [Smit et al., 2007], empirical pressure dependent equations have been formulated to adjust pump temperatures from Cases 1 through 4 to an internal pump based temperature (Case 5). Internal pump temperatures are considered to be the best approximation to the 'true' T_p. Further, lab experiments that compare piston temperatures to internal pump, or pump-based, temperatures (the latter using the empirically derived equations) found a 1-3K difference, prompting an additional equation that corrects for this temperature bias [Smit et al., 2014]. The

resultant pump temperature corrections required for each case listed in Table 2.6.1 are:

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Case 1: Equation 2.6.1

- (a) $T_{Pcase1} = 7.43 0.393 Log_{10}(P)$ $P \ge 40 \text{ hPa}$
- (b) $T_{Pcase1} = 2.7 2.6 Log_{10}(P)$ 6 < P < 40 hPa
- (b) $T_{Pcase1} = 4.5$ $P \le 6 \text{ hPa}$

835 836 Case 2, 3: Equation 2.6.2

- (a) $T_{Pcase2,3} = 20.6 6.7 Log_{10}(P)$ P > 70 hPa
- 838 (b) $T_{Pcase2.3} = 8.25$ $15 \le P \le 70 \text{ hPa}$
- 839 (c) $T_{Pcase2,3} = 3.25 4.25 Log_{10}(P)$ $5 \le P < 15 \text{ hPa}$

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Case 4: Equation 2.6.3

- 842 (a) $T_{Pcase4} = 6.4 2.14 Log_{10}(P)$ P > 40 hPa
- 843 (b) $T_{Pcase4} = 3.0$ $3 \le P \le 40 \text{ hPa}$

845 Case 5: No adjustment, i.e. T_{Pcase5}=0.0

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The additional correction to account for differences between T_{piston} and the internal pump, or pump based, temperatures is described as:

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$$T_{piston-internal} = 3.9 - 0.8 Log_{10}(P)$$

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It is recognized by GRUAN that equations 2.6.1 to 2.6.4 were derived from small statistical samples (Equation 2.6.4 from a sample of only three ECC sondes in the JOSIE chamber experiments; Figure 9 from Smit et al. [2007]). The adjustment formulae for Cases 2 and 3 were derived from a sample size of eight, while only three sondes were used to generate the Case 4 formula. Until GRUAN can conduct more detailed analyses of the biases related to different placements of the sonde thermistor, the uncertainties inherent in the small samples underlying equations 2.6.1 to 2.6.4 must be propagated through to uncertainties in the derived ozone partial pressures. Section 6.5 summarizes the pump temperature uncertainty parameters and equations and how these contribute to the ozone partial pressure uncertainty.

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The ASOPOS panel recommends that the final adjusted pump temperature, T_p , used to calculate the ozone partial pressure, should be defined as:

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Equation 2.6.5
$$T_p = T_{measured} + T_{Pcase_i} + T_{piston-internal}$$

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where $T_{measured}$ is the pump temperature recorded by the sonde, T_{Pease_i} is the correction that depends on the case, and $T_{piston-internal}$ is the additional correction defined by equation 2.6.4.

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2.7 Determining the partial ozone column above the top of flight

871 GRUAN's purpose for calculating total column ozone for each profile is to allow for

comparisons against an independent spatially and temporally co-located total column ozone

measurement to provide a means of validating the quality of the ozonesonde ozone profile. The

standard technique for computing total column ozone from an ozonesonde measurement includes

adding a climatological ozone partial column value above the balloon burst altitude. Most often,

these partial columns are based on satellite and ozonesonde observations [McPeters et al, 1997,

877 2007, 2012; Labow et al., 2015], though some sites have developed their own monthly

climatologies e.g. based on microwave radiometer-derived ozone profiles. Comparisons of the

integrated ozonesonde ozone profile plus the partial column above the top of flight can then be

made with ground-based and satellite measurements of total column ozone (e.g. Dobson

spectrophotometer, Brewer spectrometer, OMI, GOME-2).

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When integrating ozonesonde profiles within a GRUAN ozonesonde programme, that integration shall be truncated at 7 hPa since the ozone profile above 7 hPa has higher uncertainty due to the degradation of the pump efficiency (Section 2.5) and evaporative effects on the sensing solution at very low pressures [Bryan Johnson/NOAA, private communication]. It is preferable that GRUAN sites derive their own monthly climatologies of ozone partial columns above the top of the flight since these will be more relevant than the zonal mean climatologies provided by McPeters et al. [2012]. It is important that these climatologies include uncertainties so that these can be propagated through to the derived ozonesonde total column ozone uncertainty. Until site-

890 can be propagated through to the derived ozonesonde total column ozone uncertainty. Until site-

specific climatologies are available, the McPeters et al. climatologies may be used to derive the ozone partial column above the burst pressure. Where the balloon bursts at pressures higher than the McPeters et al. [2012] pressure limit of 32 hPa a total column ozone value cannot be derived and the flight total column ozone value should be recorded as a null value.. It is recognized that there may be gaps in the profile measurements due to intermittent telemetry. Profiles with large data gaps shall be identified and evaluated on a case-by-case basis and the flight total column ozone value and, importantly, its uncertainty, calculated according. The GRUAN ozonesonde data product shall include the following ozone column-related metadata:

- The integrated ozone column amount (in DU) up to 7 hPa or balloon burst, whichever is lower
- The pressure level at the top of the integration [hPa].
- The ozone partial column (in DU) above burst pressure either from the McPeters et al. [2012] climatology or from the site-specific climatology.
- If available, co-located ground-based or space-based measurements of total column ozone shall be included.

GRUAN encourages sites to include any ancillary measurements of surface and column ozone measurements in the metadata submitted to the centralized GRUAN ozonesonde data processing facility. Redundancy in ozone measurement systems provides a powerful tool for validating and evaluating the ozone measurements in any given time series.

2.8 **Dependence on the radiosonde**

processing calculations of the geopotential height.

Radiosonde pressure and temperature measurements are used to calculate the geopotential heights. Thus, radiosonde measurement errors will cause the measured ozone to be assigned incorrect altitudes and pressures. As with ozonesondes, there are a number of radiosonde manufacturers whose instruments have changed in model, material, and algorithm since the 1970's. There are measurable differences between manufacturers, i.e. Vaisala vs iMET, and between models, i.e. Vaisala RS-80 vs RS-92, that impact the ozonesonde measurement, particularly at low pressures [Smit et al., 2014; and references therein]. GRUAN shall document radiosonde manufacturer, model and type of interface so that appropriate calibrations and corrections to the pressure and temperature, as well as RH, can be made in the pre- and post-

GRUAN procedure protocol

- Calibration of the radiosonde surface pressure, temperature, RH and determination of any offset between geopotential and GPS height measurements, if and when available, shall follow the processing guidelines dictated by the GRUAN Radiosonde Technical Document (X.X.X).
- Handling biases in the geopotential height calculation in the absence of GPS measurements shall be the responsibility of the Radiosonde WG-GRUAN, task team, and Lead Centre.
- Radiosonde/Ozonesonde offsets in height and pressure, if any, shall be documented and geopotential heights shall be recalculated by the Lead Centre GOASS (refer to Section 3.7).

• Quantifying the contribution of the radiosonde uncertainty to the ozone measurements, if any, shall be the responsibility of the Radiosonde WG-GRUAN, task team, and Lead Centre.

2.9 Conversion efficiency

One of the terms in the ozone uncertainty calculation is the contribution of the uncertainty in the conversion efficiency. The conversion efficiency refers to the stoichometric factor of 1:1 assumed in the I₂:O₃ relationship. Interferences with this one-to-one relationship can arise from the buffering of the solution [Johnson et al. 2002; Vömel and Diaz, 2010]. The cathode solution contains a buffer of sodium-hydrogen phosphate to maintain the solution concentration and a neutral pH of 7.0 during flight. GRUAN shall follow a half buffered cathode solution for ENSCI sensors and a full buffer for SPC, as recommended by WMO/ASOPOS [Smit et al., 2012; 2014]. Johnson et al. [2002] performed stoichiometric sensitivity and pH tests and measured excess ozone at low pressures due to the buffering effect. This would yield a I₂:O₃ relationship larger than unity. This offset in the stoichiometry has been documented by others (Smit et al., 2014, section 3.2.2 and references therein; Johnson et al, 2002, section 2.1 and references therein). In the ozone partial pressure equation, Equation 1, the conversion efficiency is assumed to be unity and is therefore excluded from the equation. However, the uncertainty of this unity assumption can be a significant contributor to the ozone uncertainty estimates and is addressed in Section 6.6.

956 3 GRUAN OZONESONDE PROGRAMMES

- 957 The GRUAN Guide (herein referred to as GCOS-171) states that the primary objective of
- 958 GRUAN is to provide reference measurements for a range of upper-air climate variables.
- Reference quality observations are based on key concepts in metrology, in particular traceability.
- Metrological traceability is the process whereby a measurement and its uncertainty, can be
- related to a reference through a documented, unbroken chain of calibrations, each of which
- 962 contributes to the measurement error.

To provide the best measurements of ozone and its uncertainty, a detailed understanding of the instrumentation, standard operating procedures (SOPs), and data processing is required. To lend confidence in the long-term stability of the data records for a single GRUAN Ozonesonde Programme and the entire network as a whole, the instrumentation, standard operating procedures, and data processing must produce datasets that are homogenized across the entire network.

- For this reason, GRUAN ozonesonde certification applies to the overall infrastructure underlying the ozonesonde measurement and the subsequent production of a final GRUAN ozonesonde reference product. This infrastructure is defined in the present report as a GRUAN Ozonesonde Programme, and includes
- 1. the SOPs that condition and calibrate each ozonesonde instrument prior to launch,
 - 2. the mandatory collection of metadata used to characterize the singular features of each unique ozonesonde instrument,
 - 3. the acquisition of the raw data and metadata to the RSLaunchClient utility for central processing,
 - 4. the steps involved for create a final homogenized GRUAN ozonesonde product,
 - 5. the handling of storage and dissemination of all pertinent levels of ozonesonde measurements.

In order to be GRUAN-certified each GRUAN Ozonesonde Programme must include the following three mandatory components:

- 1. The GRUAN Ozonesonde Instrumentation and Measurement Report (GOIMP): A dynamic document submitted to the GRUAN Lead Centre, via email, by the GRUAN ozonesonde programme representative describing their measurement program and capabilities, as well as documentation on the history of its ozonesonde data record, if any. The GOIMP shall include all aspects of the programme such as instrumentation inventory, SOPs, measurement schedule, and up-to-date data acquisition and archiving status. Further details of what should be included in the report are addressed in Section 3.2.
- 2. Proof of the ability to provide all essential metadata and raw data to the RSLaunchClient utility: An interactive JavaScript tool designed to compile all metadata associated with each ozonesonde instrument launched (i.e. those measurements collected by the ground station data acquisition system per launch). The essential metadata is described in Section 3.6 and is upload together with the raw data by the RSLaunchClient at a designated

- GRUAN ozonesonde data handling centre for processing by the GRUAN Ozonesonde
 Analysis Software System (GOASS). All metadata uploaded by RSLaunchClient shall be
 consistent with the latest version of the GRUAN check list (found in Appendix A-1 and
 A-2 for refurbished sondes).
- 1003 3. The GRUAN Ozonesonde Analysis Software System (GOASS): A centralized data 1004 processing software collecting and analyzing in a standardized manner the raw-data of all 1005 certified GRUAN ozonesonde instruments sent out through the RSLaunchClient utility. 1006 Before processing the raw data, the GOASS reconciles the metadata received from the 1007 RSLaunchClient with those contained in the GOIMP. Any inconsistency is immediately 1008 reported, thus providing a near-real-time check of the measurement traceability and 1009 stability, as well as a quick identification of change. The output of the GOASS consists of 1010 certified GRUAN ozonesonde products of various levels designed to be used by different 1011 communities for different science applications. Individual GRUAN Ozonesonde 1012 Programmes will be audited, as well as annually reviewed in compliance with the 1013 requirements and recommendations of GCOS-171 and this present document. GRUAN Ozonesonde Programmes not in compliance all three of the mandatory components listed 1014 1015 above may lose their GRUAN certification.

1016 3.1 Site assessment and certification considerations for GRUAN Ozonesonde 1017 Programmes

Ozonesonde sites seeking to become a GRUAN Ozonesonde Programme will be subjected to the same assessment and certification process as all other sites in the network. This section provides pragmatic criteria for assessing and certifying existing and new sites. Ozonesonde sites will follow the specific requirements regarding site assessment and certification under Section 5.1 of GCOS-171.

GRUAN recognizes that sites will vary in infrastructure and financial support. In order to be compliant with the mandatory operating protocols defined in Sect. 5.3 of GCOS-171, each GRUAN Ozonesonde Programme should do the following:

- 1. Provide reference quality observations, i.e., observations characterized by a traceable calibration, a comprehensive uncertainty analysis, a readily accessible documentation, a validation through inter-comparison campaigns, and complete metadata availability.
- 2. Provide access to raw data and assure long-term storage of the raw data, as well as metadata, either at the site, at another GRUAN facility, or at another internationally accessible archive in accordance with the GRUAN Data Policy document (referred to in Section 8.2 GCOS-171).
- 3. Provide complete metadata for each measurement as defined in Section 3.6 of this document.
- 4. If available, and certainly encouraged, provide redundant reference observations of ozone from co-located ground-based instruments for independent evaluation and validation (refer to Sections 7.7 and 8.3 on parallel observations and validation, respectively).
- 5. Provide annual reports summarizing the ozonesonde operations at the site, including changes in instrumentation, how those changes were managed, and any improvements made.
- 6. Conduct the ozonesonde programme with an operational philosophy of continually striving to improve measurement accuracy (e.g., by working with other GRUAN Ozonesonde Programmes, or participating in field and laboratory experiments).
- 7. Manage change proactively as defined in Section 7 of this document.
- 8. Actively communicate with the GRUAN Lead Centre, WG-GRUAN and GRUAN Task Team for Sonde (TTS) through attendance at meetings and emails.

Specifically, GRUAN ozonesonde certification shall be assessed based on the follow criteria:

- 1. The content and completeness of the GOIMP each ozonesonde candidate site is required to file at the designated GRUAN Lead Centre (refer to Section 3.2).
- 2. The level to which the ozonesonde candidate site conforms to GRUAN prescribed SOPs consistent with WMO GAW Report 201 to guarantee homogeneity of quality across the network. Determining whether the SOPs of an existing site meet the prescribed operating protocols will be done objectively against the standards outlined in Section 3.5.
 - i. Sites that do not meet the WMO operating procedure standards can choose to adopt the prescribed SOPs in order to qualify to become a GRUAN site.
 - ii. New sites shall be expected to adopt the GRUAN prescribed SOPs.

iii. Sites that launch refurbished ECC-sensors should follow the NOAA re-conditioning SOPs in Appendix A-2 or manufacturer SOPs (refer to Section 4.5).

- 3. The level to which the ozonesonde candidate site conforms to the GRUAN prescribed conditioning and pre-flight check list whose metadata will be collected by the RSLaunchClient. Metadata requirements from the check list are addressed in Section 3.6.
- 4. The schedule frequency where a minimum of twice monthly launches spaced bi-weekly is required. This is addressed in Section 5.2. A *fully* operating GRUAN Ozonesonde Programme shall perform weekly launches. Weight shall be given to the added value each candidate site brings to the network (see Section 3.2.1 below).

3.2 GRUAN Ozonesonde Programme assessment and certification process

1074 A schematic of the site assessment and certification process is provided in Figure 2 of GCOS-1075 171.

Once a site has been identified for possible inclusion in GRUAN, through either of the routes shown in Figure 2 of GCOS-171, the following sequence of events will be used to assess the site for potential GRUAN certification:

- 1. The candidate site will be given the GRUAN manual (GCOS-171) and this ozonesonde technical document, as well as documentation describing data submission protocols and the procedures that must be followed when data are submitted to the internal GRUAN archives via the RSLaunchClient (addressed in Section 3.6).
- 2. The response from the candidate site shall be given in the form of the GOIMP submitted to the designated GRUAN Lead centre and should include:
 - 1. If it is an established GRUAN site that proposes to add an ozonesonde measurements programme or a new GRUAN site that will include an ozonesonde measurement programme.
 - 2. A complete description of how the ozonesonde measurement programme will be conducted. Such information would include launch frequency and scheduling, detailed SOPs, a copy of the check list and metadata inventory, and data storage policies. This information must be sufficient to establish the ability of the site to meet the mandatory operating protocols outlined in Sections 3.5 3.7.
 - 3. Include any cooperative agreements with other sites and institutions already in the network. This is highly desirable to ensure that expertise is disseminated to similar measurement programmes in operation at other sites.
 - 4. The management structure of the site and a general description of the manner in which the site is operated. This would include a description of current and expected future funding levels for on-going operation of the site.

5. A description of which data centres the measurements have previously been submitted to and are currently being submitted to.

- 6. A description of how past ozonesonde measurements from the site have been processed. This will be used to assess whether the time series to date meet the standards for a GRUAN reference measurement. Particularly important in this regard will be detailed documentation around how changes in SOPs over the history of the measurement programmes have been managed to derive a homogeneous time series of measurements.
- 7. A description of past metadata data records and storage. This will be used to assess whether the time series to date meet the traceability standards for a GRUAN reference measurement.
- 8. A list of the ozonesonde experts employed at the site who would likely participate in the analyses of the data collected within GRUAN. This may include mention of experts at partnering scientific organizations.
- 3. There is likely to be some iteration between the Lead Centre and the candidate site to confirm specific details, fill in information gaps, and finalize the documentation from the candidate site.
- 4. Based on the documentation received from the candidate site, the Lead Centre will then write a short recommendation. This, together with the documentation from the candidate site, will then be submitted to the WG-GRUAN who will evaluate the proposal within 6 calendar months against the requirements listed in Sections 3.5, 3.6, and 4. One or more visits to the site by members of the WG and/or Lead Centre within this 6-month period may be required to obtain specific additional information about the measurement programmes slated for inclusion in GRUAN at that site. If accepted, these measurement programmes will then be included in the GRUAN certification for the site.
- 5. Regardless of the outcome, the WG-GRUAN and Lead Centre will provide written constructive feedback to the candidate site outlining strengths and weaknesses of their programme for GRUAN purposes and suggestions as to future improvements for GRUAN operational purposes. This feedback is non-binding but rather intended to provide useful guidance and support to site capability development and retention of current capabilities.
- **6.** Annual reports shall summarize GRUAN operations at the site identifying any changes in ECC or radiosonde instrumentation, scheduling, procedures, equipment, and improvements. The intent of the annual report is to ensure that SOPs developed for the network have been adhered to, and to identify changes that may require additional reprocessing that is not already taken into account or require re-assessment of GRUAN certification. These reports will be presented at annual GRUAN meetings.

3.2.1 Criteria for assessing added value

The GRUAN Ozonesonde Programme assessment and certification process follows closely the more general GRUAN site certification process described in Section 5.5 of the GCOS-171. Once a site has committed to operating a set of measurement programmes under the protocols defined in Section 5.3 of GCOS-171, the added value that an ozonesonde site brings to the GRUAN network will be assessed according to:

- The extent to which the ozonesonde site can fulfill the measurement programme expected of a fully equipped GRUAN site (Section 3.1). Achieving all of the measurement programme requirements is not mandatory for the inclusion of a site in GRUAN. However, the extent to which a site can meet these requirements will determine, in part, the additional value that that site brings to the network. For example, ozonesonde sites located in a large region of the globe containing no other GRUAN Ozonesonde Programmes and making the minimum required bi-weekly launches will be assessed as adding as much value to the network as a site making weekly reference quality measurements but located very close to another GRUAN ozonesonde site. These high priority measurement programmes will be refined as the research which forms their basis progresses. This documentation will be updated to reflect scientific requirements.
 - The extent to which the ozonesonde site provides profiles measurements of ozone in regions of atmospheric phenomena which were not previously sampled. In this case, the added value will depend on the locations and capabilities of the sites already participating in the network.
 - The extent to which the ozonesonde site brings unique observational and/or analysis capabilities aligned with GRUAN scientific objectives to the network as a whole and the likelihood of being able to propagate those capabilities across other sites in the network.
 - The extent to which the ozonesonde site is prepared to forgo locally established operating procedures and adhere to the SOPs established by the Lead Centre and adopted by the majority of the sites already in the network. Unwillingness or inability to do this would count against a site in the assessment of the added value it would bring to the network.
 - The availability of historical measurements that conform to the GRUAN standard. All else being equal, a candidate site that extends an existing multi-decadal time series of reference quality measurements will be assessed as adding more value to the network than a site that would initiate the same measurement programme starting at the present. Detailed documentation in the GOIMP would be required describing how changes in SOPs, instruments, calibration procedures, data processing algorithms and operators over the history of the measurement programmes have been managed to ensure that the historical measurements are reference quality. Where historical reference quality measurements are available, consideration will be given by the WG-GRUAN and Lead Centre to providing these as GRUAN data through the GRUAN data archives.
 - The extent to which the ozonesonde site can commit to a multi-decade programme of measurements. While it is recognized that a multi-decade programme of measurements cannot be guaranteed, a statement of intent with documented support (e.g. from the host institution or relevant funding agency) will add to the assessment of the value that the site brings to the network.
 - The extent to which the ozonesonde site can provide redundant observations of the priority 1 and ECVs or can conduct periodic inter-comparisons and laboratory studies.

- The extent to which a site is capable of measuring other ECVs identified in GCOS-112 as being desired quantities.
- The level of institutional support for the site and commitment to maintaining long-term reference quality measurement programmes. If, in addition, a site can demonstrate that it is actively pursuing resources to enhance its capability, such as the addition of new measurement programmes, this would also enhance the added value the site would bring to the network. It is also desirable that there is full host institution commitment to GRUAN-related activities and that this commitment is not dependent on a single individual.
 - The level of institutional support for the site (and any partner institutions) to undertake fundamental scientific research of the measurements from the site and other GRUAN sites. Because GRUAN includes aspects of both operational and research networks, a strong and ongoing science programme is required to ensure that GRUAN fulfills its role as a research network.
- The degree of historical or planned cooperation with other sites both within and outside the GRUAN network including other GRUAN-relevant networks e.g. NDACC,
 SHADOZ, GAW, and WOUDC.
- 1203 Such assessments of added value shall rely on the expert judgement of the WG-GRUAN and
- Lead Centre, recognize the heterogeneity of the sites within the network, and facilitate a practical
- approach to expansion of the network following the 2009-2013 implementation phase for
- 1206 GRUAN (GCOS-134) and it amendments.
- 1207 Determining optimal locations for GRUAN sites as part of added-value assessment to ensure that
- the needs of the user community are met shall consider the following:
- 1209 1. Covers a major climate region.
- 1210 2. Covers a region of large atmospheric modes, e.g. ENSO, SAM, OBO
- 1211 3. Environment, e.g. tropics, mountainous, dessert, island
- 4. Spatial co-location with other Ozonesonde Programmes

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3.3 GRUAN Ozonesonde Training Programme

- 1215 Operational uncertainty includes uncertainties related to instrument set-up and operation. To
- reduce operational uncertainty, and in line with Section 1.4 of GCOS-171, the Lead Centre and
- 1217 WG-GRUAN shall identify Ozonesonde Programmes where instrument operators need training
- on GRUAN ozonesonde SOPs, and shall organize cost-efficient training courses for those
- 1219 operators at appropriate locations to encourage uniformity of ozonesonde instrument operation
- between sites. At least one staff member of a GRUAN Ozonesonde Programme should be in
- attendance to an initial training session in which the GRUAN-specific ozonesonde best
- measurement practices and the use of RSLaunchClient are taught. The GRUAN Ozonesonde
- 1223 Programme representative shall be one of the trained staff.
- 1224 In addition to training at the time of certification, training is required for any new measurement
- scientist joining the ozonesonde programme team. Though training may be done through other

- existing members of staff, it is strongly recommended that a GRUAN training session be
- provided at a GRUAN site where optimal standard operating procedures are kept up-to-date.
- 1228 If WG members deem that a potential candidate requires training, or an existing GRUAN
- Ozonesonde Programme requires re-training, GRUAN will try to partner the site organization
- 1230 with an ozonesonde expert who can do a site visit for training or re-training. The Lead Centre
- require that at least one member of the WG-GRUAN is an ozonesonde expert. An ozonesonde
- expert includes operators of a GRUAN Ozonesonde Programme, members of ASOPOS, or other
- ozonesonde experts that have participated in JOSIE studies and ozonesonde inter-comparison
- 1234 field campaigns. Thus, although not required, re-training may be done by an ozonesonde expert
- 1235 within the WG-GRUAN.
- 1236 For those GRUAN Ozonesonde Programmes already partnered with ozonesonde launch experts,
- training and maintaining up-to-date practices shall be coordinated between the two partners.
- 1238 Sites that require re-training will be determined by these means:
 - A GRUAN site makes a formal written request for re-training to the Lead Centre.
- When the WG-GRUAN concludes that upon reviewing a sites annual report that retraining is necessary to guarantee consistency of quality.
- An audit, addressed in Section 3.10, reveals deficiencies in the operating procedures that necessitate re-training to maintain GRUAN certification.

3.4 GRUAN Ozonesonde Programme data management

General considerations shall be drawn from Section 8 of GCOS-171.

3.4.1 Overview of the data flow

Refer to Figure 3 of GCOS-171 which shows a schematic representation of the flow of data in GRUAN to the user community.

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- 1250 GRUAN data levels *relevant to ozonesondes* are based on the GRUAN Data Management 1251 Manual:
 - Level 0 (L0): Original primary raw data (PRD). This is the 'rawest' form of data available before any processing has been applied, i.e., the raw data slices acquired by the data acquisition electronics
 - Level 1 (L1): Converted raw data (CRD). These data are stored in a common well-described file format intended for long-term storage. They are pre-processed raw data and might already represent parameters to be used in end-user's application
 - Level 2 (L2): Standard GRUAN product data (SGPD) resulting from all processing steps associated with a single instrument.

- Measurements and metadata are bound together in each of these data levels. PRD are ingested
- 1262 from all GRUAN sites into the internal GRUAN data archive hosted at the Lead Centre. Direct
- exchange of PRD between sites is discouraged since this circumvents the data versioning
- protocols and reduction of the raw data to a common CRD file format. Similarly, direct exchange
- of CRD between sites is discouraged since this circumvents network wide application of

corrections, re-processing, and homogenization techniques applied to convert CRD to SGDP that would be implemented at the Lead Centres' data processing facility.

From PRD data submission to processing, storing and dissemination of SGPD

- 1. Level 0 ozonesonde raw data (PRD) and metadata, listed in Section 3.6, shall be collected by the RSLaunchClient utility.
- 2. A complete list of the essential and desirable PRD is found in Table 3.1 of this section.
- 3. A complete list of the essential and desirable metadata is found in Table 3.4 of this section
 - 4. Each GRUAN site is responsible for storing the PRD and associated metadata in it's original format and in digital format.
 - 5. The PRD shall be saved as Level 1 converted raw data (CRD) via the RSLaunchClient.
 - 6. Processing of the ozonesonde raw data will be held in the designated GRUAN internal data archive at the Lead Centre.
 - 7. The Lead Centre GOASS will be responsible for using the CRD and essential metadata to create the final standard ozone products (SGPD), as outlined in Section 3.7.
 - 8. A complete list of SGPD are found in Table 3.2 of this section.
 - 9. A designated GRUAN Lead Centre storage facility shall be responsible for archiving and maintaining the ozonesonde metadata, CRD, and SGPD for all Ozonesonde Programmes.
 - 10. The SGPD, including their metadata and documentation, will be provided to the user community through the external GRUAN data archive hosted at NCEI.

Processing of the CRD, held in the GRUAN internal data archive, to produce SGPD will occur at the designated Lead Centre central processing facility. This processing should include applying the necessary corrections, and uncertainty estimates in a consistent and traceable manner across identical instruments from other Ozonesonde Programmes. The SGPD, including their metadata and documentation, are provided to the user community through the external GRUAN data archive currently hosted at NCEI. A performance monitoring process (see Section 9 of GCOS-171), implemented at the Lead Centre, will provide feedback on performance to individual sites.

3.4.2 GRUAN data policy

Since GRUAN is co-sponsored by WMO, GRUAN ozonesonde data dissemination and use shall comply with WMO Resolution 40 (Cg-XII) which calls for free and unrestricted international exchange of data. Refer to Section 8.2 of GCOS-171 for further details on the data dissemination and exchange policy.

3.4.3 Collation of Metadata

- Essential and desirable metadata are listed in Section 3.6.1. Metadata will be submitted via the RSLaunchClient utility and archived at the designated GRUAN Lead Centre and NCEI.
- "Desirable" metadata defined in Section 3.6.1 are not required and the RSLaunchClient will not reject profiles if these desirable variables are excluded.

1308 Metadata should not preclude information derived from historical documents such as observing 1309 practices manuals, site inspection reports, government policies, resource and funding 1310 programmes. 1311 1312 Management and maintenance of metadata requires the investment of resources. Present day 1313 technology for database warehousing of digitized metadata has the added benefit that metadata 1314 can be accessed, linked to measurements, and easily transferred. To facilitate metadata collation, 1315 the RSLaunchClient utility will be responsible for ingesting as much metadata as possible to be 1316 saved and stored at a designated GRUAN archive. Ozonesonde Programmes are required to keep 1317 original copies of their metadata at their own storage facility, as secondary storage back-up. 1318 1319 Metadata documents related to historical operations at GRUAN sites and to historical data 1320 archives should be inventoried and properly conserved until such time as their information 1321 content can be transferred to a medium which supports multiple users' access and conforms to 1322 GRUAN reference measurement guidelines. 1323 1324 Metadata needs to have the same level of commitment as observed data. Incomplete, outdated, or 1325 inaccurate metadata can be as detrimental, indeed in some cases worse, than no metadata at all. 1326 Regular reviews of metadata content for confirmation and accuracy should be part of regular 1327 GRUAN operations. Support to investigate new metadata sources, information management 1328 technologies and information sharing capabilities should be on-going in an effort to make

accessible and preserve the historical investment in the data collected.

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1332	3.4.4 Ozonesonde Data Products
1333	The Ozonesonde Primary Raw Data (PRD)
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1335	Each ozonesonde launched generates an array of measurements captured by the ground station
1336	data acquisition system. The PRD generally measures, but is not limited in measuring, the
1337	following variables listed in Table 3.1. The essential data variables listed are the basic
1338	fundamental data variables that are to be collected by the RSLaunchClient. The RSLaunchClient
1339	will collect and manage uploaded ozonesonde PRD to the designated GRUAN Lead Centre. All
1340	the PRD shall be saved to a Level 1 converted raw data (CRD) file for archiving at the
1341	designated GRUAN Lead Centre storage facility and processing shall be done by the GOASS
1342	addressed in Section 3.7 to create the SGDP. Desirable PRD (in blue) is not required input to the
1343	RSLaunchClient and profile data will not reject if these desirable variables are excluded.
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1345	Table 3.1 Essential and Desirable Ozonesonde Primary Raw Data (PRD) variables
1346	
1347	16. Time [min]
1348	17. Time GMT [hh:mm:ss]
1349	18. Pressure [hPa]
1350	19. Geopotential height [gpm]
1351	20. Temperature [K]
1352	21. Relative Humidity [%]
1353	22. Ozone Partial Pressure [mPa]
1354	23. Ozone Mixing Ratio per volume [ppm]
1355	24. Horizontal Wind Direction [decimal degrees] (range: 0:360)
1356	25. Horizontal Wind Speed [m/s]
1357	26. GPS Geometric Height [m]
1358	27. GPS Longitude [decimal degrees] (range: -180:+180)
1359	28. GPS Latitude [decimal degrees]
1360	29. GPS Satellites
1361	30. GPS Time GMT [hh:mm:ss]
1362	31. GPS Pressure [hPa]
1363	32. Internal Temperature [K] (box or pump)
1364	33. Ozone Current [μA]
1365	34. Battery Voltage [V]
1366	35. Pump Current [μA]
1367	36. Rise Rate [m/s]
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1369	The Ozonesonde Standard GRUAN Data Product (SGDP)
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1371	Each PRD should be archived at the same vertical and temporal resolution. Thus, each

ozonesonde profile shall archive SDPG at the same vertical and temporal resolution. The 1372

GOASS shall use the PRD, in conjunction with the metadata also collected from the 1373

RSLaunchClient, to generate the ozonesonde SGPD. Section 3.7 goes through the GOASS steps 1374 1375

required to generate the ozonesonde SGPD from the CRD. The family of ozonesonde SGPD are

- listed in Table 3.2. Apart from the uncertainty estimates, it is not mandatory for all variables
- under the ozonesonde SGDP family to be measured. For example, heritage ozonesonde
- measurements used radiosondes that did not have the means or capability of acquiring GPS information.

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Table 3.2 Collection of Ozonesonde SGPD

- 1382
- 1383 1. Time [min]
- 1384 2. Radiosonde Pressure [hPa]
- 1385 3. Radiosonde Pressure Offset [hPa]
- 4. Geopotential height [gpm]
- 1387 5. RadiosondeTemperature [K]
- 1388 6. Radiosonde Temperature Offset [K]
- 7. Radiosonde Relative Humidity [%]
- 1390 8. Radiosonde RH offset [%]
- 9. Ozone Partial Pressure [mPa] using Equation 2.6.5
- 1392 10. Ozone Partial Pressure uncertainty [%] using Equation 6.5.2
- 1393 11. Ozone Partial Pressure [mPa] using Equation 2.6.6
- 1394 12. Ozone Partial Pressure uncertainty [%] using Equation 6.5.1
- 13. Ozone Mixing Ratio per volume [ppm] using (9) of this list.
- 1396 14. Ozone Mixing Ratio per volume [ppm] using (11) of this list.
- 1397 15. Radiosonde Horizontal Wind Direction [decimal degrees] (range: 0:360)
- 1398 16. Radiosonde Horizontal Wind Speed [m/s]
- 1399 17. Radiosonde GPS Geometric Height [m]
- 1400 18. Radiosonde GPS Longitude [decimal degrees] (range: -180:+180)
- 1401 19. Radiosonde GPS Latitude [decimal degrees]
- 1402 20. Internal Temperature [K] (box or pump)
- 1403 21. Ozone Current [μA]
- 1404 22. Ozone Current and background contribution (Section 6.2)
- 1405 23. Ozonesonde Pump Flow rate. Φ (Section 6.3).
- 24. Ozonesonde Pump Correction Factor, Ψ, (Section 6.4).
- 1407 25. Ozonesonde Pump Temperature, T_p (Section 6.5).
- 26. Ozonesonde Conversion efficiency, η (Section 6.6).
- 1409 27. Radiosonde Pressure and Temperature offset uncertainty [defined and addressed in the GRUAN Radiosonde Technical Report (X.X.X)]
- 1411 28. Total Column Ozonesonde (TCO) [DU]
- 1412 29. Pressure above which the TCO is calculated [hPa]
- 1413 30. Partial column ozone above (29) [DU]

1414

- 1415 As seen from Table 3.2, uncertainty estimates shall form part of the ozonesonde SGDP
- 1416 collective. The Lead Centre GOASS shall be responsible for calculating these estimates
- 1417 addressed in detail in Section 6. The measurement uncertainty describes the current best
- 1418 knowledge of instrument performance under the conditions encountered during an observation
- and therefore merits its own separate listing in Table 3.3 below.

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Table 3.3 Uncertainty variables as part of the ozonesonde SGPD.

1422	1. Ozone partial pressure uncertainty (Section 6.1).
1423	2. Ozone Current and background contribution (Section 6.2)
1424	3. Pump Flow rate, Φ (Section 6.3).
1425	4. Pump Correction Factor, Ψ, (Section 6.4).
1426	5. Pump Temperature, T _P (Section 6.5).
1427	6. Conversion efficiency, η (Section 6.6).
1428	7. Radiosonde Pressure and Temperature uncertainty. These values will be calculated
1429	according to the GRUAN Radiosonde Technical Report (X.X.X)
1430	
1431	
1432	
1433	3.4.5 File naming convention
1434	The filename convention described here is taken from Section 2.1 of the Manual for the Data
1435	Management in GRUAN [GRUAN-TD-1 DRAFT v0.3v0.3 (2010-132010-07-13)] and will
1436	apply for metadata XML files and for the CRD and SGPD data files in the designated GRUAN
1437	Lead Centres file archive. The obligatory parts of the file names should be:
1438	
1439	 Unique Station Identifier → GAW ID and station location name, i.e.
1440	NRB_Nairobi_Kenya
1441	 Data level → number
1442	 Data product level → CRD or SGPD (not used for metadata file naming)
1443	 Version of data product → number
1444	 Date / Time → in universal standard time (UTC)
1445	 Date / Time of the creation of CRD and SGPD files
1446	• Identification of the specific instrument → 'ECCSonde'
1447	• Identification of central tracer → 'Ozone'
1448	3.4.6 Data format
1449	 Metadata will be provided to the end-user in XML format.
1450	 CRD and SGPD will be stored in CSV ASCII format. SGPD will be provided to the
1451	NCEI in that format. ASCII format is an accepted standard output used by the leading
1452	ozonesonde archiving centers (SHADOZ, NDACC, and WOUDC).
1453	3.4.7 Data dissemination
1454	
1455	• Users of GRUAN data shall have access not only to the measurements and their
1456	uncertainties, but also to the metadata information which includes instrument
1457	specifications, operating procedures, data algorithms used, and when changes to any of
1458	these occurred through the complete time period of the data set.
1459	• Users shall have access to previous versions of the ozonesonde SGDP.
1460	3.4.8. Data archiving

- The ozonesonde metadata, CRD and SGPD are expected to be stored at the nominated GRUAN central data processing facility Lead Centre.
 - A designated GRUAN storage facility should be established. This would:
 - Allow the Lead Centre to maintain statistics on data usage. This would be useful when applying for funding to support GRUAN operations.
 - Allow users of data to be informed if and when newer versions of the data become available.
 - Facilitate reporting of potential errors, flags, and anomalies in the data by end-users.
 - GRUAN sites shall be responsible for storing their PRD.
 - The metadata and SGPD shall be made available at the NCEI.
 - Ozonesonde data dissemination shall comply with the data policy guidelines in Section 8.2 of GCOS-171.
 - It is important that the GRUAN archive includes all previous versions of any given data set so that analyses using previous versions of data can be repeated if required.

3.4.9 **Data gaps**

GRUAN recognizes that there may be gaps in the profile measurements due to telemetry interference.

- 1. **Profiles should not be excluded if data gaps occur.** There is useful data extending from the surface up to the lower stratosphere, i.e. around 35 km or 5 hPa, that satisfies the four key user groups of GRUAN data products. From Section 1.2 of GCOS-171 they are the (i) climate detection and attribution community, (ii) satellite community, (iii) The atmospheric process studies community, and (iv) numerical weather prediction (NWP) community. Depending on where the data gaps occur and the extent of these data gaps, there remains useable quality reference data that can still satisfy one or more of these four communities. However, the satellite community will be the most affected by data gaps.
- 1. Profiles with very large and intermittent data gaps should be identified and evaluated in the annual reports and periodic audits. Ultimately, it is up to the end-user to determine whether the data gaps should be excluded from their study.

3.5 The GRUAN Standard Operating Procedures

GRUAN seeks to ensure that all sites operate to the same reference quality standard to guarantee homogeneity of quality across the network. JOSIE and BESOS demonstrated that changes of an ozonesonde instrument (e.g. different manufacturers) or operating procedures (e.g. incorrect choice of sensing solutions, incomplete metadata, missing procedures) can have a large impact on sonde data quality and thus influence the trends derived from such records. ASOPOS demonstrated that after standardization and homogenization improvement of precision and accuracy by about factor 2 might be gained. The JOSIE-1996 results show that differences between the ECC ozone sensors types are largely due to differences in the preparation and correction procedures applied by the different sites [Smit et al., 2000]. The WMO/GAW SOPs are designed to reduce random errors by maintaining consistent and reproducible ozonesonde

measurements. Standardization of the SOPs has been shown to improve the precision and 1506 accuracy to less than $\pm 5\%$, while non uniformity in SOPs will lead to inhomogeneities in the time series and between station data records [Smit et al, 2007, Deshler et al, 2008].

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GRUAN protocol

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1511 GRUAN strongly recommends that Ozonesonde Programmes use the WMO/GAW ozonesonde 1512 conditioning and preparation procedures outlined in detail in Annex A of GAW Report No. 201.

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- Associated with the SOPs is a check list to help ensure that the site operators follows the
- 1515 WMO/GAW ozonesonde conditioning and preparations procedures in a consistent manner. The
- 1516 GRUAN check list (Appendix A-1) has been designed to be a guide to certify that SOPs are
- 1517 being followed correctly. It is strongly recommended that potential site candidates use the
- 1518 GRUAN check list in place their own SOPs, but it is not required as long as sites can
- 1519 demonstrate that WMO/GAW SOPs are being followed and all essential metadata are recorded.

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Refurbished Sonde SOPs

- 1522 Refurbished sensors must follow more rigorous conditioning and testing. The ASOPOS panel
- 1523 concluded that at present it is not clear in how often recovered ozonesondes can be re-used after
- 1524 reconditioning. Currently there are no quality assurance standards for refurbished sensors and a
- number of ozonesonde sites fly refurbished sondes using their own set of SOPs. Sites risk 1525
- 1526 potentially introducing artifacts in the data records if the re-conditioning procedures are not done
- 1527 properly. A basic set of SOPs for refurbished sensors can be found in Appendix A-2, although
- 1528 manufacturer SOPs should not be discounted. Further discussion on refurbished sensors can be
- 1529 found in Section 4.5. GRUAN strongly recommends and encourages that JOSIE studies.
- independent laboratory tests, and inter-comparison field measurements be conducted to establish 1530
- 1531 SOPs for refurbished sondes that GRUAN can draw on to incorporate across the Ozonesonde
- 1532 Programme network.

3.6 The RSLaunchClient Utility 1533

- 1534 The RSLaunchClient utility will collect and manage uploaded metadata and ozonesonde PRD to
- 1535 the GRUAN Lead Centre. Specifically, GRUAN Ozonesonde Programmes will be required to
- 1536 provide essential metadata and PRD to the RSLaunchClient. GRUAN defines essential data as
- 1537 input requirements to the RSLaunchClient. If one of the basic essential metadata variables is
- 1538 missing a flag will be given or, in some cases, the entire profile will be rejected (e.g. if a
- 1539 metadata variable required to calculate an uncertainty estimate is missing). Because each
- 1540 ozonesonde ECC sensor is considered a new instrument it is essential that every singular feature
- 1541 of each sensor is documented. The metadata represents all the characteristics that define each
- 1542 unique ozonesonde and will be collected by the RSLaunchClient. Most of the metadata shall be
- 1543 taken from the check list that has been designed to follow the WMO/GAW SOPs. The GRUAN
- 1544 check lists for new and refurbished ozonesondes are provided in Appendix A-1 and A-2. The red
- font in the check lists indicates that it is essential RSLaunchClient metadata. It is strongly 1545
- 1546 recommended that potential sites use the GRUAN check list in place of the manufacturer check list.

1549 3.6.1 Metadata for RSLaunchClient

- 1550 To provide the best evaluation for the ozonesonde measurement uncertainty, a detailed
- understanding of the instrumentation is required for the conditions under which it is used. The
- ozonesonde metadata summarizes the unique characteristics of each ozonesonde instrument in
- response to standard operational procedures, and it makes all factors that contribute to the
- measurements traceable. Following the WMO/GAW SOPs a list of essential and desirable
- metadata has been designed and is provided in Table 3.4 below. Desirable metadata (in blue) is
- not required input to the RSLaunchClient. Profiles shall not be discounted if desirable metadata
- is not included.
- 1558 1559
- Table 3.4 Essential and Desirable metadata variables specific to ECC sensors
- 1560
- 1561 1. Station Name
- 1562 2. GAW Number
- 3. Site Latitude [decimal deg (range -90:+90)]
- 4. Site Longitude [decimal deg (range -180:+180)]
- 5. Site Elevation [m]
- 6. Re-conditioned Sonde: Y or N. If Y then the following information is required:
- 1. Date flown (YYYYMMDD)
- 1568 2. Date found (YYYYMMDD)
- 1569 3. Date returned (YYYYMMDD)
- 4. Date stored on shelf until ready for the 3-7 day pre-condition (YYYYMMDD)
- 5. Comments on overall ozonesonde/pump condition
- 6. 100 ppbv calibrated source current [μA]
- 7. 100 ppbv ECC-sensor current [μA]
- 8. Zero Ozone air calibrated source current [μA]
- 9. Zero Ozone air ECC-sensor current [uA]
- 7. Date of Initial Pre-conditioning or Re-conditioning (done at least 3 days prior to flight):
 YYYYMMDD
- 1578 8. Date of Secondary Preconditioning (if done): YYYYMMDD
- 9. Launch Date: YYYYMMDD
- 1580 10. Launch time [GMT]: HH:MM:SS
- 1581 11. Sonde Type and Serial Number
- 1582 12. Radiosonde Type and Serial Number
- 1583 13. Interface Type and Serial Number
- 1584 14. Ground station system and software version
- 1585 15. Pump current [μA]
- 1586 16. Pump Pressure [psi]
- 1587 17. Pump Vacuum [in Hg]
- 1588 18. Zero Ozone Source
- 1589 19. KI Solution Strength [%]
- 1590 20. Buffer amount
- 1591 21. Volume of cathode sensing solution [cm³]
- 1592 22. IB0
- 1593 23. IB1

- 1594 24. IB2
- 1595 25. Initial preparation Response Time [μ A/sec] = Time for ozone to drop from 4-1.5 microA
- 26. Initial preparation current after Response Time [μA]
- 1597 27. Flow rate: All 5 flow rates [sec/100ml]
- 1598 28. Flow rate average [sec/100ml]
- 29. Lab Temperature during Flow rate test [degC]
- 1600 30. Lab RH during Flow rate test [%]
- 1601 31. Lab Pressure during Flow rate test [hPa]
- 32. Surface Pressure at launch site [hPa]
- 33. Surface Temperature at launch site [degC]
- 1604 34. Surface RH at launch site [%]
- 35. Surface Wind Direction at launch site [deg]
- 36. Surface Wind Speed at launch site [m/s]
- 1607 37. Inverse pump efficiencies factors
- 1608 38. Balloon Brand
- 39. Balloon Pay-off Weight [grams]
- 40. Independent measurements of total column ozone.
- 1611 41. Dobson or Brewer or other instrumentation to be defined in Section 8.3.
- Variables specific to the radiosonde data stream, such as P-T-U calibrations, offsets, and
- uncertainty calculations, shall borrow from the Radiosonde Analysis Software in the GRUAN
- 1615 Radiosonde Technical Document (X.X.X).

1616 3.7 The GRUAN Ozonesonde Analysis Software System (GOASS)

- 1617 The GRUAN Ozonesonde Analysis Software System (GOASS) is the centralized data
- processing software that shall analyses the PRD of all certified GRUAN Ozonesonde
- Programmes sent out through the RSLaunchClient utility. Before processing the PRD, the
- 1620 GOASS reconciles the metadata received from the RSLaunchClient with those contained in the
- 1621 GOIMP. Any inconsistency is immediately reported, thus providing a near-real-time check of the
- measurement traceability and stability, as well as a quick identification of change. The GOASS
- must be transparent, i.e., must be developed and optimized in consultation with all GRUAN
- Ozonesonde Programme Representatives/investigators, as well as the GRUAN Lead Centre,
- 1625 WG-GRUAN, and TTS. These investigators shall meet regularly to discuss the implementation
- of updates to the GOASS, and whether processing changes pertain to one or all of the GRUAN
- Ozonesonde Programmes. The output of the GOASS consists of certified ozonesonde metadata,
- 1628 CRD, and SGDP defined in Sections 3.5 and 3.6.

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The basic principles driving the technical programming of the GOASS are as follows:

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- 1. Each GRUAN ozonesonde instrument shall be considered as a unique instrument within the network.
- 2. Each GRUAN ozonesonde may experience instrumentation change over time.
- Each GRUAN ozonesonde shall use up-to-date SOPs recommended by WMO/GAW
 across the network.

- 1638 The need for centralized processing therefore implies a very stringent data processing approach.
- 1639 The GOASS must integrate correction methods and associated uncertainties that are accepted by
- 1640 GRUAN and user communities as being appropriate for the science application foreseen. It is
- therefore the GRUAN Lead Centre, TTS, and GRUAN Ozonesonde Programme
- Representative's joint responsibility to develop and maintain the operational GOASS. Failure of
- 1643 GRUAN Ozonesonde Programmes to use an operational version of the RSLaunchClient and
- 1644 GOASS will result in delivery delays of the ozonesonde SGDP, and therefore can result in the
- cancelation of the Programme's certification at the time of its audit.

The PRD and associated metadata accepted by the RSLaunchClient will be processed by the Lead Centre using the GRUAN Ozonesonde Analysis Software System (GOASS). The GOASS shall perform the following steps to transform the PRD to the final Level 2 GRUAN standard ozonesonde product (SGDP) (defined in this Document as a collection of profile measurements of ozone, meteorological variables from the radiosonde and uncertainties):

1. Apply filtering criteria to test the performance of an individual ECC sensor, summarized in Table 3.5 below. Aspects of the conditioning process should fit within the following specific thresholds. GRUAN site operators shall use these threshold criteria to gauge the quality of the ECC sensor and perform repeat tests if necessary to bring the ECC sensor into compliance. Ideally, ozonesonde raw data should not be uploaded to the RSLaunchClient if certain threshold criteria are violated.

Table 3.5 Threshold criteria for ECC ozonesondes used by the RSLaunchClient to test the performance quality of each sensor. These are specifically for SPC and ENSCI sensor types.

Test Indicator	Threshold Criteria	Action if violated
Average pump flow rate	Within 26-36 sec/ml	Flag and record in metadata
Response Time	20-30 sec	Flag and record in metadata
Pump temperature	273-315 K (-15 – 40 C)	Flag for ozonesonde datum exceeding threshold.
Background I _{B0}	0-0.05 μΑ	See 1.1
Background I _{B1}	0-0.1μΑ	Flag and record in metadata
Background I _{B2}	0-0.1 μΑ	Flag and record in metadata
Background I _B	Should be I_{B0} or the minimum of I_{B0} , I_{B1} , and I_{B2} if $I_{B0} > 0.05$ μA	See 1.1
Pump motor current	> 100 μA for SPC, > 90 μA for ENSCI	Flag and record in metadata
Pump pressure	> 10 psi	Flag and record in metadata
Pump vacuum	< 20 in Hg	Flag and record in metadata
KI Solution	0.5% buffered for ENSCI; 1.0% buffered for SPC	Should be always be correct for GRUAN certification. For historic data, where applicable, transfer functions shall be applied.
Pump Correction Factors (PCF)	Komhyr [1986] values for SPC-6A and Komhyr et al. [1995] values for ENSCI	Ozone values shall be recalculated using the correct (PCF)

- 1.1 I_{B0} shall be used as the final background, I_B , in the ozone equation (addressed in Section 2.2). For the case where $I_{B0} > 0.05~\mu A$ GOASS shall recalculate ozone using the minimum of I_{B0} , I_{B1} , and I_{B2} as I_B . If that minimum background current exceeds the 0.05 μA threshold then GOASS shall recalculate ozone using I_B =0.05 μA shall be used and flagged in the metadata. It should be recorded in the metadata which background is used as I_B .
- 2. GOASS shall apply the RH correction, C_{PH} , explained in detail in Section 2.4. The final flow rate, Φ =(mean flow rate)• C_{PH} , shall be used in Equation 2.1.1 to calculate the Level 2 ozone partial pressure product.
- 3. Radiosonde/Ozonesonde offsets in height and pressure, if any, shall be documented in the metadata and geopotential heights shall be recalculated, in accordance with the GRUAN Radiosonde Technical Document (X.X.X).
- 4. Adjusted pump temperatures using Equation 2.6.5 and sub-equations shall be calculated. That along with the measured pump temperatures shall be used to calculate two ozone partial pressures.

- 5. After the above corrections are applied ozone partial pressure shall be recalculated using Section 2.1 Equation 1 in two ways: (i) using the original measured pump temperature and (ii) the adjusted pump temperature based on bullet 4 above.
- 6. Uncertainties for each measured parameter in the ozone partial pressure equation shall be calculated and are defined in the subsections of Section 6.
- 7. The individual uncertainties shall be used to calculate the ozone partial pressure for each ozone datum, as defined in Section 6.1.
 - **8.** A total column product shall then be calculated based on the processing protocol defined in Section 2.7.

1687 Flagged Data

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- Data that are not within threshold levels itemized in Table 3.5 shall not be rejected but must be
- 1689 flagged and documented in the final archived metadata. Flagged metadata shall be included as a
- diagnostic tool in each GRUAN Ozonesonde Programmes annual report. Audits shall use the
- statistics gathered on flagged metadata and the SGDP to help evaluate the continuity of GRUAN
- 1692 Ozonesonde Programmes.

3.8 GRUAN ozonesonde calibration management

- Ozonesonde ground stations generally do not require calibration at the manufacturing,
- instrumentation, or operational levels. Calibration of the ECC sensor comes from adhering to the
- 1696 SOPs and completing the metadata check list requirements. The results of the conditioning
- procedures summarizes the unique responses of the individual sonde to a standard fixed set of
- operating procedures. At the time of this document, there is no precedent or standard rules that
- 1699 requires sites to test or calibrate aspects of the ground station equipment, nor is there a
- mechanism to ensure equipment standards and quality. It would ideal to establish guidelines by
- 1701 which a GRUAN Ozonesonde Programme can calibrate its ground station equipment such that
- sources of error and uncertainty can be further identified, traced, and included as part of the
- 1703 uncertainty budget for ozonesondes.

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World Calibration Facility for Ozonesondes (WCFOS)

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- 1707 The World Calibration Center for Ozonesondes (WCCOS) at the Forchungszentrum, Jülich,
- 1708 Germany periodically conducts inter-comparison experiments (JOSIE) to establish and maintain
- 1709 quality assurance of the ozonesondes sensors. JOSIE performs routine testing of existing and
- 1710 newly manufactured ECC ozone sensors to (i) check the instrument performance in a controlled
- environment, (ii) maintain up-to-date SOPs, (iii) test individual ECC sensor capabilities, and (iv)
- develop uncertainty estimates for the individual instrument parameters. The WG-GRUAN shall
- use findings from the JOSIE reports to evaluate current best practices and whether changes to the
- ozonesonde SOPs or processing procedures need to change. Members of the WG-GRUAN are
- encouraged to participate in JOSIE initiatives to keep abreast of new findings. It is highly
- desirable for GRUAN sites to endorse and participate in JOSIE-led activities.
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1718 Calibration of the ozonizer test unit

- 1720 The ozonizer used to condition and prepare an ECC sensor does not generate a traceable amount
- of ozone. Comparisons against an independent calibrated reference, such as a TEI surface ozone
- monitor, to generate a known ozone amount would be very useful. It would be desirable for sites
- to provide traceable ground/instrument checks, such as a surface ozone monitor (e.g. TEI) at the
- time of each profile measurement, prior to launch and independent of the manufacturer. In the
- case of refurbished ECC sensors it is strongly recommended that a calibrated source of ozone to
- test the instrument performance be used and included as part of their SOPs.

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3.9 Ozonesonde Programme versioning system

- 1729 A system of traceable version numbers and dates for all GRUAN Ozonesonde Programmes shall
- be developed to allow for a full identification and tracking of changes in SOPs, and data
- processing since the initial certification. Every reprocessing of the metadata, CRD, and SGDP
- must be reflected in an increment in the data version and an update to the date of creation by the
- 1733 GOASS (see file naming convention in Section 3.4.5) as prescribed in the data versioning
- 1734 protocols developed by the GRUAN Lead Centre. Such data updates must also be communicated
- to users who have accessed earlier versions of the data and who have voluntarily registered to
- 1736 receive notifications of such data updates (see Section 8.6 of GCOS-171). For this reason it is
- also important that all older versions of any data set are always archived and made available
- through the GRUAN Lead Centre's archive.

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3.10 GRUAN Ozonesonde Programme auditing

- 1741 Certification of GRUAN sites will not be a single event. GRUAN sites will be audited by
- members of the WG-GRUAN at 3-4 year intervals to ensure that the programme continues to
- 1743 meet GRUAN standards.

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1745 The audit will involve:

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- 1. A review of the sites annual reports.
- 2. An ozonesonde launch in front of WG-GRUAN auditors that demonstrates that the SOPs are being followed in accordance with Section 3.5.
 - 3. Check lists will be reviewed against the GRUAN Check lists if not used.
 - 4. Discussions with the scientists responsible for the measurement programmes at the site.
 - 5. In the eventuality of identified site problems the following protocols shall be followed (taken from Section 5.6 of the GCOS-171):
 - 1. Should a measurement programme at an existing GRUAN site show significantly reduced observational capability over more than a year, as evaluated by the criteria listed above, the WG-GRUAN and Lead Centre shall investigate the circumstances at that site, and, if needed, exclude that programme from the GRUAN certification for that site. The WG-GRUAN and Lead Centre shall work proactively with sites to resurrect such programmes providing training, technical and in-kind support as practical and as needed.
 - 2. Should the overall contribution of a site be deemed sufficiently diminished to call into question its continued presence in the network, the site shall be informed immediately

in writing. The site shall be given six months to form a capabilities recovery plan, in consultation with the Lead Centre and WG-GRUAN. Should this plan be accepted the site will have no more than two calendar years from its acceptance to implement agreed key aspects. In the eventuality that this is not achieved, the site shall be suspended with an invitation to submit anew at such a time as problems are remedied.

- 3. An existing GRUAN site may also request the temporary suspension of some or all of the measurement programmes at that site from GRUAN certification. This could occur for example in cases of unforeseen budget limitations, non-availability of personnel or some other unavoidable circumstance affecting the measurement programmes at the site. Such a request must be submitted in writing to the WG-GRUAN and the Lead Centre. At some later time, should the site request recertification of those measurement programmes previously suspended, the procedure for certification as outlined in Figure 2 of GCOS-171 shall be followed.
- 4. A certified GRUAN Ozonesonde Programme may also request a temporary suspension of its certification. This could occur, for example, in case of unforeseen budget limitations, non-availability of personnel or some other unavoidable circumstance affecting the measurement programme. Such a request must be submitted in writing to the WG-GRUAN, Lead Centre, TTS. The normal procedure for certification should be followed if re-certification is later requested.

Along with the cooperation and goodwill of participating sites, nations, and individuals, the establishment of these GRUAN site assessment and certification guidelines provides one of the main foundations for ensuring that GRUAN meets its goals as a climate observing network.

1786 4 GRUAN OZONESONDE INSTRUMENTATION

- As described in Section 2 (and elsewhere) of the GCOS-171, one key requirement of GRUAN instruments is to provide reference measurements, i.e., using principles based on key concepts in
- 1789 metrology such as (but not limited to) traceability. Traceability must apply at all levels of the
- data acquisition and processing chain, including instrumentation. Therefore to ensure full
- traceability, a complete and accurate description of each certified GRUAN Ozonesonde
- Programme system must be provided in GOIMP (defined in Section 3.2). An entire ozonesonde system comprises the following components:

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- 1. Electrochemical concentration cell (ECC) ozonesonde which is encased in a molded polystyrene weatherproof box for ascent into the lower stratosphere
- 2. Radiosonde
- 3. Interface electronics, if applicable, to couple the ECC ozonesonde to the radiosonde.
- 4. A ground station for receiving data provided by the radiosonde manufacturer. The ground station consists of a portable, tripod mounted, antenna with built-in pre-amplifier, and a long coaxial cable that connects the antenna to a 403 MHz receiver.
- 5. A laptop with pre-installed data acquisition and processing software. This allows data to be received and processed during the balloon flight.
- 6. A 1200 baud modem that connects the laptop to the 403 MHz receiver.

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Refer to the GRUAN Radiosonde Technical Report (X.X.X) for instrument details pertaining to radiosondes and their ground stations and data acquisition systems. Refer to the ECC manuals for information pertaining to the materials and electronics of the ECC sensor mainframe, and type interface circuitry which couples the sensor to the particular type of meteorological radiosonde [e.g. DMT, 2014; SPC, 1999].

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- The requirements and recommendations on ozonesonde instrumentation provided in this section apply only to the ozonesonde techniques recognized to be mature enough to be providing reference measurements of ECVs of highest-enough priority for GRUAN. As of this document, these include the SPC and ENSCI instruments coupled with the Vaisala and iMET radiosondes and ground stations and associated data acquisition and processing software. Other radiosonde
- and ground station data acquisition system packages, addressed in Section 4.4, shall be included
- as they are assessed and recognized by the Lead Centre and WG-GRUAN to be providing
- products compliant with GRUAN measurement standards. It is important to mention that
- 1820 GRUAN shall not prescribe any instrumentation system and setup in particular. Rather, GRUAN
- shall provide simple and practical recommendations that encourage sites to use the best practices
- in full compliance with the requirements and recommendations detailed in this Guide.

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4.1 General considerations from Section 6.1 of the GRUAN Guide to Operations (GCOS-171)

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- Periodic reviews of ozonesonde instrumentation likely to be of use within GRUAN shall be
- undertaken. It must also be recognized that not all Ozonesonde Programmes within GRUAN will

- operate the same ozonesonde instrumentation and ground station system. GRUAN will not
- prescribe the use of specific ozonesonde instruments and ground station systems in the network
- since the emphasis is not on prescribing an instrument, but rather on prescribing the capabilities
- required of an instrument and allowing individual sites to select an instrument that achieves those
- capabilities. That selection will be influenced by the requirements and recommendations put
- 1834 forth by this document, and other scientific, programmatic, and practical constraints on the site.
- 1835 That said, the fewer the number of different types of instruments and measurement techniques
- deployed within and among GRUAN Ozonesonde Programmes, the more likely network
- 1837 homogeneity will be achieved.

A number of criteria should be considered when selecting ECC ozone sensor instruments for use in GRUAN including: instrument heritage (i.e. maturity), sustainability, robustness of measurement uncertainty, and manufacturer support.

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Since 1996, the Forchungszentrum, Jülich, Germany has been the site of the WCCOS. The first Jülich Ozone Sonde Inter-comparison Experiment (JOSIE) (1996) has shown that ECC ozone sensors that performed with the best precision and accuracy were the Science Pump Corporation (SPC) and ENSCI instrument manufacturers [Smit et al., 2000]. The 1996 experiment calculated a precision to within ±(3-4)% and an accuracy to within ±(4-5)%. Subsequent JOSIE-led activities have included both types of ECC sensors in their inter-comparisons.

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GRUAN recognizes that ECC sensor technology is constantly evolving and that not all sites within GRUAN will operate the same ECC sensor, e.g. a new site may decide to adopt a new ECC-sensor that has not been yet been included in JOSIE studies, or an existing site may continue to use an older manufacturing model or obsolete sensing solution (e.g. 2% unbuffered) to avoid potentially introducing a discontinuity in the measurement time series.

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4.1.1 Instrument Selection

- 1857 As of this Document there are two ECC sensors on the market:
 - a. Science Pump Corporation (SPC)
- 1859 b. ENSCI

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- 1. Both manufacturer types are considered the leading industry standard for ECC ozonesondes and have a long heritage of launches.
- 2. The commercial demand for SPC and ENSCI is sufficient to support the production and use of the instrument for the expected multi-decade deployment within GRUAN.
- 3. There is no reason to suspect that both instrument manufacturers will stop production in the foreseeable future, even if a newer (but not necessarily better) instrument is developed and marketed.
- 4. All ozonesonde stations with long-term ECC records use one or both types and are archived at SHADOZ, NDACC, and the WOUDC.
- 5. Finally, all WMO-supported ECC inter-comparison studies (JOSIE), campaigns (BESOS) and other laboratory and field studies have included these two manufacturing types. Thus, there is a substantial body of literature documenting its performance and measurement uncertainty.

6. Through JOSIE and independent dual-launch studies, the precision and accuracy claims for both instruments and its resultant data is sufficiently robust and meets the uncertainty and stability standards under Section 4.1 of GCOS-171.

In the event that a new ECC ozone sensor is commercially developed, GRUAN expects the manufacturer to (i) actively participate in JOSIE and other instrument inter-comparisons, (ii) be willing to disclose the necessary information required to form a fully traceable chain of sources of measurement uncertainty in accordance with the GCOS-171 mandatory operating requirements, and (iii) make available the algorithms used for corrections within the data processing software to conduct uncertainty analysis. In accordance with GCOS-171 guidelines, it is a 'fundamental requirement that the information required to reprocess the data at any time in the future must be made available (though not necessarily publicly available)'.

4.2 Measurement Redundancy

"Having different instruments at GRUAN sites measuring the same atmospheric parameters will be invaluable for identifying, understanding and reducing systematic effects in measurements"

- GCOS-171

Examples of redundant instruments that measure profile ozone are the ozone Lidar and Microwave Radiometer. Other ozone monitoring instruments to consider that can complement ozonesonde profile measurements are the TEI surface ozone monitor, and UV Vis instrumentation. All these instruments can provide uninterrupted hours of measurements at one given location. Unlike these fixed located instruments, balloon-borne ozonesondes provide insitu measurements at varying locations and altitudes with time. The challenge therefore is to match the ozonesonde altitude and time with those other instruments with careful considerations about the geographic displacement from the ground-based instrument site. Section 6.4.2. of GCOS-171 provides an overview of the characteristics of Lidar and microwave instrumentation. Methods on resolving the time/altitude differences from these instruments shall draw on information found in the GRUAN technical documents for Lidar and Microwave Radiometers. GRUAN shall draw on methods developed by Calisesi et al. [2005], Bodeker et al. [2013], Hassler et al., [2008] and references therein, that create site atmospheric state best estimates (SASBE) of ozone profiles from combining ozone instrumentation of varying temporal and spacial resolutions to provide objective evaluation of ozonesonde performance. Ozonesonde

4.3 The SCIENCE PUMP CORPORATION ozonesonde

- 1910 The earliest Science Pump Corporation (SPC) ECC ozonesonde measurements occurred in the
- late 1960's [Komhyr, 1969]. Table 1 from Johnson et al. [2002] summarizes the model
- 1912 production dates and design changes from the earliest SPC design (SPC-1A). The first known
- 1913 operating guidelines for preparing ozonesondes for flight was created for the now retired SPC-
- 1914 4A model in the NOAA technical memorandum [Komhyr, 1986]. The current manual has been
- optimized for the SPC-6A model design [SPC Manual, 1999].

measurements themselves may be part of SASBE.

GRUAN protocol procedure

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- 1919 As of this document, the GOASS shall process PRD from SPC-4A models and higher to produce
- 1920 the ozonesonde SGDP using procedure protocols established in this document. All other historic
- 1921 SPC profiles from older SPC models should be inventoried and properly conserved until such
- 1922 time as their information content can be evaluated, assessed, and assigned uncertainty estimates
- that conform to GRUAN reference standards and guidelines.

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- 1925 While the SPC modifications over time improved ECC performance, error characterization in
- 1926 models older than SPC-4A are not as well known. The first SOP manual was conceived with the
- 1927 SPC-4A model design in mind and changed with model design as they were altered to optimize
- 1928 performance. Given that these older SPC models no longer exist and are no longer flown, JOSIE-
- 1929 type studies or campaigns are necessary to determine error estimates or empirical corrections to
- 1930 all historic instrumental parameters.

4.4 The ENSCI ozonesonde

- 1932 ENSCI Corporation started in the late 1980's with similar ECC sensor instrument configuration
- to that of the SPC-5A model (refer to Table 1 of Johnson et al., [2002]). Komhyr [1997]
- 1934 published the first ENSCI operations handbook for the 2Z model. There is no significant
- instrumental differences between the Z and 2Z models [Bryan Johnson/NOAA, personal
- 1936 communication]. The Z model is configured to be compatible with interface boards of other
- 1937 ground station systems (e.g. Vaisala) while the 2Z has a built-in V7 interface board compatible
- 1938 with the iMET ground station.
- 1939 Since the late 2000's Droplet Measurement Technologies (DMT) took over the manufacturing of
- 1940 ENSCI ECCs. The model design has remained unaltered at the helm of DMT, thus GRUAN does
- 1941 not make a distinction between the two companies. As of this document, the most up to date
- 1942 ENSCI manual has been published by DMT [2014] and includes much of the WMO/GAW SOP
- 1943 recommendations and protocols. As of this Document, ENSCI has separated from DMT and is
- 1944 once again it's own manufacturing entity.

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GRUAN protocol procedure

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The GRUAN archive shall accept ENSCI Z, 2Z ozonesonde instrument profiles to produce the ozonesonde SGDP.

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4.5 A typical GRUAN ozonesonde data acquisition systems

- 1952 The ozonesonde is interfaced with a radiosonde and uses its data acquisition system to transmit
- and record the ozone current and other parameters that calculate the ozone partial pressure (see
- 1954 Equation 1 in Section 2.1). The ozonesonde/radiosonde equipment and data acquisition system
- shall also be referred to as the 'ozonesonde ground station'. From to Section 6.1 of GCOS-171

- "GRUAN will not prescribe the use of specific instruments in the network since the
- emphasis is not on prescribing an instrument, but rather on prescribing the capabilities

required of an instrument and allowing individual sites to select an instrument that achieves those capabilities."

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As of this Document, there are a number of ozonesonde/radiosonde ground station systems operating with varying degree of publicly available documentation. These include Vaisala (Finland), iMET (USA), Lockheed-Martin-Sippican (LMS, USA), Meisei (Japan), Modem (France), and Chang Feng (China). The Vaisala type ground station system is the most commonly used, having a heritage of long term records of ozonesonde and radiosonde measurements. Specific to radiosondes there is a large body of literature that have characterized the uncertainties and biases among the Vaisala models (Dirksen et al., [2014] and references therein; Hurst et al. [2011]; Nash et al. [2006; 2011]; Steinbracht et al., [2008] and references therein; and Vömel et al. [2007]). Hurst et al. [2011] and Stauffer et al [2014] were among the first inter-comparison studies of iMET and Vaisala models. Both iMET and Vaisala adhere to the instrument selection requirements addressed in Section 6.1 in GCOS-171. This includes, but is not limited to, information content, instrument heritage (e.g., maturity), sustainability (e.g. sufficient commercial demand), robustness of measurement uncertainty, and manufacturer support. Both ozonesonde ground station systems are known to provide all the essential raw data and metadata listed in Tables 3.1 and 3.4, respectively

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As of this Document, there is varying degree of documentation that is publicly available on the other supporting ozonesonde/radiosonde ground station systems mentioned above. However, meeting the GCOS-171 instrument selection criteria and GRUAN data quality assurance and measurement standard policies can be assured provided that the manufacturer is:

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• Committed to improving the performance of its instrument.

1984 • Willing to provide essential GRUAN raw data and metadata listed in Tables 3.1 and 3.4, 1985 respectively. 1986

 Prepared to actively participate in instrument inter-comparisons (e.g. JOSIE) and field campaigns (e.g. BESOS).

Willing to disclose the necessary information required to form a fully traceable chain of sources of measurement uncertainty (e.g. releasing SOPs and algorithms used for any corrections within its data processing software).

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GRUAN procedure protocol

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- 1. At a minimum, GRUAN requires that candidate sites use ground stations that provide the essential metadata (Table 3.4) and raw data (Table 3.1). These parameters are critical to characterizing each individual ozonesonde.
- 2. GRUAN shall encourage all ozonesonde/radiosonde ground station manufacturers to participate in JOSIE-led activities.
- 3. GRUAN shall encourage ozonesonde/radiosonde ground station manufacturers to provide documentation on laboratory and dual sonde launches to demonstrate that the precision and accuracy fits within $\pm (3-4)\%$ and $\pm (4-5)\%$ of the JOSIE results, respectively. These results have been determined by Smit et al. [2000] using the leading SPC and ENSCI ECC sensors (see Section 4.1.1).

4.6 Refurbished Ozonesondes

The ASOPOS panel concluded that at present it is not clear in how often recovered ozonesondes can be re-used after reconditioning. The general recommendation by the ASOPOS panel is not to fly re-used ECC-sondes, however, for a number of ozonesonde sites it is the most cost-effective way to the ensure financial stability of their programme and maintain their ozonesonde launch schedule. GRUAN shall (i) encourage sites at unique locations (refer to Section 3.2.1 on added-value criteria) that regularly launch re-used sondes to apply to become a GRUAN site and (ii) not prohibit existing Ozonesonde Programmes from including data from refurbished ozonesondes. provided that all operating conditions set forth by this Document are met.

Refurbished sensors falls under one of the "9 items" under managing changes in Section 7 of this report. Thus, established GRUAN Ozonesonde Programmes that wish to include refurbished sensors falls under the guidelines of a "change event" and programmes shall follow steps in Section 7.1 to include refurbished ozonesondes into their programme. For new candidate sites seeking to become a GRUAN site this information should be included as part of their GOIMP.

For individual GRUAN Ozonesonde Programmes re-using ECC-sensors, the re-conditioning SOPs of recovered sondes should be done by well-skilled and trained personnel and be done in such a way that the resulting metadata is always within the threshold criteria defined in Table 3.5 and does not introduce artifacts in their long term ozone records. For refurbished ozonesondes it is recommended that Ozonesonde Programmes following the modified NOAA prescribed reconditioning instructions found in Appendix A-2 or re-conditioning procedures as given by the sensor-specific manufacturer.

In recognition of the heterogeneity of the GRUAN ozonesonde network, the WG-GRUAN and GRUAN Lead Centre shall evaluate individual candidate sites ability to launch refurbished sondes based on the following

• Sites seeking to become a GRUAN site will first be assessed according to their ability to meet the mandatory operating protocols defined in Section 5.3 of GCOS-171 and specifically 3.1 of this report, and then according to the added value they bring to the network, as defined in Section 3.2.1 of this document. This will enable candidate sites to operate their ozonesonde programme to GRUAN standards.

• In assessing the value a specific site adds to the network, the WG-GRUAN and Lead Centre will base decisions on sound scientific research while exercising its discretion in evaluating the proposal against the criteria defined in value-added assessment in Section 3.2.1 of this document. Consideration shall be given to, but not be limited to, the following:

Body of peer-reviewed literature using refurbished sondes.

Historical data – sites with long term homogenous data records is a desirable factor.

• Operation set-up

 The ability and skill of site operators to re-condition sensors following re-conditioning operating protocols (Appendix A-2 or manufacturer specific).

- 2048 The availability of an ozone calibrator to assess the performance of each re-used sensor.
 - Funding constraints.

• Launch schedule which is a defining factor in assessing the extent to which the candidate site can become a fully operational GRUAN Ozonesonde Programme.

GRUAN Ozonesonde Programmes shall be responsible for conducting tests to ensure that the continuity of the data record is not compromised. Sites must clearly demonstrate that each refurbished ozonesonde is measuring ozone with an accuracy and uncertainty similar to that of a new ozonesonde. This can be done using calibrated ozone instrumentation, e.g. TEI, that tests the sensor performance against known quantities of ozone, and through duel sonde intercomparisons.

2062 5 OZONESONDE MEASUREMENT SCHEDULING

- As detailed in Section 5.2.1 of GCOS-171, a fully equipped GRUAN site is required to make
- 2064 weekly ozone profile measurements. While it is not stipulated whether such measurements
- should be made using ozonesondes, lidar or microwave radiometer, the expectation is that an
- 2066 ozonesonde measurement programme would be a staple of an GRUAN vertical ozone profile
- 2067 measurement programme.

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- Scientifically, measurement scheduling for GRUAN ozonesonde programmes is likely to be driven by:
- The needs of the stratospheric ozone change detection community. Ozonesonde flights need to be made sufficiently frequently to provide ozone time series suitable for detecting trends in the vertical distribution of ozone.
 - The needs of the air quality assessment community. Because ozone is a component of urban air quality, ozonesonde measurements need to be made sufficiently frequently to support air quality process studies.
- The needs of the satellite validation community. To the extent possible ozonesonde launches should be timed to coincide with overpasses of satellite which are also making measurements of the vertical profile of ozone.
- 2079 Ozonesonde protocols will continue to develop over time and, in the case of conflict between
- 2080 GCOS-171 guidelines and this Ozonesonde Technical Document, the schedule outlined in this
- 2081 Document shall take precedence (see Section 7.5 of GCOS-171).

5.1 General considerations from Section 7 of the GRUAN Guide

Responsibilities

The candidate site shall work with the WG-GRUAN and assigned TTS to define
 measurement schedule that allow the resultant ozone data products to best capture all important scales of temporal variability, both for trend analysis and for process

understanding.

- In designing the Ozonesonde Programmes measurement schedule it will be necessary for the TTS and WG-GRUAN to work closely with individual sites since scheduling is likely to be site specific. For example, some sites are more likely to (i) experience specific or unique atmospheric conditions related to the understanding of associated processes compared to other sites, (ii) be more financially constrained compared to other sites, and (iii) experience limit operating capabilities compared to other sites.
- These schedules should be conservative in the early stages of GRUAN because schedules will vary and depend on both the system being sampled (e.g. greater sampling being required in seasons of greater variability) and financial constraints (e.g. the costs of expendables). Thus, it is important to consider the added value of a site to the GRUAN ozonesonde network (see Section 3.2.1).
- Given that task teams have a finite operating life, should the TTS no longer exist, this scheduling guidance responsibility shall fall to selected members of the WG-GRUAN who may include participants from the wider GRUAN community to assist with revising measurement scheduling protocols.

Guiding Principles

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- Where available, scientific and statistical studies shall inform the process for establishing
 ozonesonde measurement schedules. However, a sound scientific basis for the
 measurement schedules discussed in this Document and in the GRUAN Guide to
 Operations may not always available and until they become available, the measurement
 schedules must be considered to be preliminary.
- The timing of an ozonesonde launch may be shifted to coincide with a satellite overpass and in this way provide valuable high quality data for satellite validation. This will serve the high priority satellite community.
- Where possible, measurement schedules for redundant systems should be synchronized so as to avoid sampling biases when combining the measurements into a single data product.
- Required measurement schedules may vary regionally and seasonally. In places and seasons where the parameter being measured is more variable, measurements should ideally be made more frequently.
- Factors affecting trend detection: The magnitude of the variability, the autocorrelation, the random error on the measurements, and the size and seasonality of the expected ozone trends are the factors influencing the quality of trend detection that should guide the development of measurement schedules
- Measurement scheduling shall remain stable unless there is a clear requirement for change, which would then have to be agreed with the relevant GRUAN sites.

 Amendments to the GRUAN measurement scheduling protocol shall follow guidelines outlined in Section 7.1 of this report.

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- 2129 Ozonesonde sites vary in levels of maturity (length of operation), resource (launch frequency),
- 2130 and possess varying levels of infrastructure (air-conditioned versus ambient laboratory
- 2131 conditions) and financial support (piece-meal, intermittent, or core funding). Consideration will
- be given to sites with limited funding to operate at the optimal launch frequency determined by
- 2133 the task team.

5.2 GRUAN ozonesonde measurement scheduling

- Ozonesondes are classified as ancillary measurements that provide complementary priority 1
- 2136 ECV measurements of temperature, pressure and water vapor, and priority 2 ECV measurements
- 2137 of ozone in the troposphere and lower stratosphere. All ECC-sensors considered in this report are
- 2138 considered to be research-grade instruments. To date, measuring ozone at a fixed high vertical
- 2139 resolutions with high precision can only be done by ozonesondes. Thus, it is highly desirable to
- 2140 include GRUAN ozonesonde data records to service end-user communities define in Section 1.2.

- 2142 Measurement scheduling for GRUAN ozonesondes is driven by one main factor: financial
- support for expendables which include the ozonesonde, interface electronics, and the balloon
- 2144 payload. Each ozonesonde is considered a unique instrument and generally, once an ozonesonde
- 2145 is launched it is lost. It is not common for sites to retrieve, re-condition, and re-launch the same
- sensor. Geography, land restrictions, weather, and additional resources can prohibit such rescue
- 2147 attempts. Schedules will depend upon available expendables and so there cannot be a "one-size
- 2148 fits all" solution.

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- In seeking a practical balance between sites with funding constraints and GRUAN scientific goals, GRUAN shall accept a minimum requirement of two times per
- month launches to be spaced every other week. Sites seeking to become GRUAN sites shall first be assessed according to their ability to meet the mandatory operating protocols
- defined in Section 5.3 of GCOS-171 and then according to the added value they bring to
- the network, as defined in Section 3.2.1.
- 1. A **fully** equipped GRUAN ozonesonde site shall make weekly launches. If and when possible, GRUAN shall encourage candidate or newly certified sites to become a fully equipped GRUAN site.
- 2. Sites shall upload metadata and PRD to the RSLaunchClient as soon as the launch is complete and that site has successfully archived their metadata and PRD.
 - 3. Sites shall commit to launching at around the same time of day. This is to maintain the representativeness and homogeneity of the data record. Variable ozonesonde launch times may affect the accuracy of trend assessments [Thompson et al., 2014].
 - 4. To the extent possible, ozonesonde launches should be timed to coincide with satellite overpass times that measure total column ozone and/or vertical profiles of ozone.
 - 5. Weather permitting, GRUAN advises launching the same day for bi-monthly to weekly sounding schedules. Altering a planned launch date due to inclement weather such as a natural disaster, strong winds, heavy rains, and storms that would impede a successful launch is expected. Altered scheduled launches shall be included as part of the annual report summaries.
 - 6. Where possible, measurement schedules for redundant systems should be synchronized so as to avoid sampling biases when combining the measurements into a single data product.

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5.3 Raw data acquisition and archiving

- 2176 The rawest form of ozonesonde data (PRD) acquired within a certified GRUAN ozonesonde
- 2177 programme and leading to the production of certified GRUAN data products is subject to all
- 2178 articles of the GRUAN data management policy described in Section 8 of GCOS-171, and
- 2179 adapted specifically for the ozonesondes in Section 3.4.

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- 2181 The ozonesonde PRD acquisition procedure should follow the optimal SOPs defined in
- 2182 Section 3.5. The essential raw data and metadata per ozonesonde launch shall then be uploaded
- 2183 to the RSLaunchClient (See Tables 3.4 and 3.1 for the lists of essential and metadata and PRD,
- 2184 respectively).

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- 2186 The raw data (PRD) format and metadata shall be in ASCII text and the RSLaunchClient shall
- be responsible for converting the PRD to Level 1 converted raw data files (CRD) for processing
- by the GOASS described in Section 3.7 to create the GRUAN standard product (SGDP).

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Raw data (PRD) sampling

Vertical range: 1-2 second raw data with no averaging.

Temporal range: As defined in Section 5.2 a minimum of bi-weekly launches will be accepted, although weekly launches are the ideal and encouraged.

GRUAN Ozonesonde Programmes PRD are expected to be archived in perpetuity at the site where the measurements took place, and must be uploaded as soon as the launch cycle is complete onto the designated centralized GRUAN ozonesonde data handling facility. The upload

procedure must be performed using the mandatory RSLaunchClient utility. No PRD data shall be accepted if they are not uploaded through the RSLaunchClient utility. If one or several changes of instrumentation or operating procedure occurred during a given 24 hours cycle, the PRD must be uploaded separately for each of the multiple uninterrupted data acquisition periods, each of these periods shall be considered as a separate GRUAN ozonesonde observation. Each GRUAN

Ozonesonde Programme should have included in their certification application a full description

of the local storing location and an overview of the raw data format.

2206 6 DATA PROCESSING AND UNCERTAINTY BUDGET

- 2207 The measurement uncertainty of the ozonesonde system describes the current best knowledge of
- 2208 instrument performance under the conditions encountered during an observation. This section
- 2209 summarizes how the centralized GRUAN Ozonesonde Analysis Software System (GOASS)
- 2210 processes the raw ozonesonde data (PRD/CRD) to produce a GRUAN ozonesonde standard data
- product (SGDP).

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- 2213 The assessment of the uncertainty budget of ozone measured from ozonesondes is a complex
- 2214 task. Measurement uncertainties in ozonesondes should, in the first instance, be characterized in
- the laboratory. In the past, JOSIE (Jülich Ozonesonde Inter-comparison Experiment) has played
- 2216 a key role in describing/analyzing all sources of measurement uncertainty to the extent possible,
- 2217 quantifying/synthesizing the contribution of each source of uncertainty to the total measurement
- 2218 uncertainty, and verifying that the derived net uncertainty is a faithful representation of the true
- 2219 uncertainty and is in agreement with the required (expected) target uncertainty. However, results
- from laboratory studies should be corroborated with field campaigns which are likely to test the
- sondes in an environment closer to their standard operating environment e.g. the BESOS
- 2222 (Balloon Experiment on Standards for Ozonesondes) campaign (Deshler et al., 2008). While it
- 2223 may be necessary to GRUAN to conduct laboratory studies and/or field campaigns to resolve
- operational issues specific to the use of ozonesondes within GRUAN, the GRUAN ozonesonde
- community must, wherever possible, collaborate with other international ozonesonde
- 2226 communities such as GAW, NDACC and SHADOZ whenever they are conducting laboratory
- studies and/or field campaigns.

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- With regards to the BM and CI type sondes it shall be the responsibility of the Lead Centre and
- 2230 the WG-GRUAN to evaluate the appropriateness of uncertainty estimates and determine if BM
- 2231 and CI data records are of sufficient quality to meet the GRUAN reference measurement
- standards (see Section 8 on Quality Management).

6.1 The Ozone uncertainty equation: Principles and rationale

- 2234 Since the 1990's tests conducted by JOSIE-led experiments, campaigns such as BESOS, and dual
- 2235 flight experiments have clearly demonstrated the need to characterize singular features of the
- 2236 ECC ozone sensors and standardize measurements. These activities have lead to the creation of
- 2237 the ASOPOS panel whose goals are to (i) standardizing the ozonesonde conditioning and
- 2238 preparation procedures, (ii) establishing guidelines for the reprocessing and homogenization of
- 2239 ozonesonde data records, and (iii) determining the contributions of the individual uncertainties
- of the different instrumental parameters to the ozone measurement. The WMO/GAW Report 201
- 2241 is a comprehensive summary of the ASOPOS findings and is the foundation on which GRUAN
- has used to established this technical report. The treatment of uncertainty in the GRUAN
- 2243 ozonesonde data processing will follow the recommendations and definitions of the WMO/GAW
- Report 201. These uncertainty parameters are part of the ozonesonde SGPD.

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The Ozone Uncertainty Equation

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GRUAN shall adopt the WMO/GAW ozone uncertainty equation taken from Equation E-3-2 in Smit et al, [2014]). It is written as follows:

2251

2252 Eqn. 6.1.1

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 $2254 \qquad \frac{\Delta P_{O3}}{P_{O3}} = \sqrt{\frac{\left(\Delta I_M\right)^2 + \left(\Delta I_B\right)^2}{\left(I_M + I_B\right)^2} + \left(\frac{\Delta \eta_C}{\eta_C}\right)^2 + \left(\frac{\Delta \Phi_P}{\Phi_P}\right)^2 + \left(\frac{\Delta T_P}{T_P}\right)^2 + \left(\frac{\Delta \Psi}{\Psi}\right)^2}$

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- where the term, $\left[\left(\Delta I_{M}\right)^{2}+\left(\Delta I_{B}\right)^{2}\right]/\left(I_{M}+I_{B}\right)^{2}$ is the contribution of the uncertainty in
- background current, the $(\Delta \eta_c / \eta_c)^2$ term is the contribution of the conversion efficiency
- 2259 uncertainty, the $(\Delta \Phi_P / \Phi_P)^2$ term is the pump flow rate uncertainty, the $(\Delta T_P / T_P)^2$ term is the
- 2260 contribution of the pump temperature, and the $(\Delta\Psi/\Psi)^2$ term is the pump flow correction factor
- 2261 uncertainties. Equation 6.1.1 is the sum of the squares of the uncertainty in each term of the
- ozone partial pressure equation (Section 2.1, Eqn. 1). The uncertainties are assumed to be
- random and gaussian and therefore follow the gaussian law of error propagation. Each
- 2264 instrumental uncertainty term is defined in subsequent sections.

6.2 Contribution of the uncertainty in background current

- 2266 The term $\left[\left(\Delta I_{M}\right)^{2}+\left(\Delta I_{B}\right)^{2}\right]/\left(I_{M}+I_{B}\right)^{2}$ from equation 6.1.1 is the contribution of the uncertainty
- 2267 in background current, where ΔI_M is the uncertainty in the measured current, I_M , and ΔI_B is the
- 2268 uncertainty in the background current, I_B.

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- 2270 There is no standard or statistically robust method for estimating the uncertainty of the
- 2271 background current. JOSIE experiments used small sample sizes, less than 14 ECC sensors, to
- 2272 conduct the background current experiments published in Smit et al, [2007] and ultimately used
- in the WMO/ASOPOS guidelines [Smit et al, 2012; 2014]. Results from Table 7 of Smit et al.
- 2274 [2007] record an average I_{B0} measurement ('background current before O₃-exposure') and 1-
- sigma uncertainty of 0.02±0.02 μA using ENSCI sensors with a 0.5% half buffer KI solution and
- 2276 0.023±0.013 μA using Science Pump Corporation (SPC) sensors with a 1.0% full buffer KI
- solution.

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- 2279 Based on the JOSIE results above, GRUAN will adopt a $\pm 0.02~\mu A$ background current
- 2280 uncertainty, ΔI_B , for ENSCI 0.5% half buffer KI solution and a $\pm 0.013~\mu A$ uncertainty for
- 2281 Science Pump ECC 1.0% full buffer KI solution because there are no other uncertainty estimates
- 2282 for I_{B0} in the literature. Furthermore, there is the added complication that this is a single
- 2283 measurement per unique ECC sensor so uncertainties cannot be be directly ascertained.

The uncertainty in the ozone current, ΔI_M , shall be set to 0.1 μA which is the resolution of the digital interface board (Terry Deshler/UWy and Herman Smit/Forchungszentrum, personal communication).

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2289 The uncertainty constants are summarize in Table 6.2.1 below.

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Table 6.2.1 Constants in the ozone current uncertainties

ECC Sensor	$\Delta I_{ m M}$	ΔI_{B}
ENSCI/0.5%		±0.02 μΑ
SPC/1.0%	μA , and $\pm 0.01 \mu A$ for currents below 1 μA .	±0.013 μΑ

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Background uncertainties outside the ENSCI/0.5% and SCP/1% pairing shall have to undergo similar rigorous testing to establish uncertainty estimates. In this case, profiles shall be stored in CRD format until such time as background uncertainties can be establish and applied to create the ozonesonde SGDP. SGDP cannot be generated unless all uncertainty contributions to ozone

2298 in Equation 6.1. are known.

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6.3 Contribution of the uncertainty in pump flow rate

- From Section 2.4 Equation 2.4.1 the final mean flow rate is corrected for the humidification
- effect, C_{PH} , and differences between the internal pump temperature and the ambient air, C_{PL} .
- The uncertainty associated with the determination of the mean flow rate is the ratio of the standard deviation of the five flow rates to the square root of the sample population, which in this
- 2306 case is five. The equation is expressed as

2307

2308 Equation 6.3.1
$$\Delta T_{100} = \frac{\sigma_{T100}}{\sqrt{N}} \text{ where N=5}$$

2309

2310 This equation is based on error analysis by Bevington and Robinson [1992] (Chapters 3 and 4).

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The uncertainty in C_{PH} and C_{PL} are site specific. For existing sites that have established at least one year's worth of ozonesonde launches, i.e. a minimum of 24 total launches, relative uncertainties, ΔC_{PH} and ΔC_{PL} , shall be calculated in the following way

2315

2316 Equation 6.3.2 $\Delta C_{PH} = \frac{\sigma_{CPH}}{\sqrt{N_{CPH}}}, \ \Delta C_{PL} = \frac{\sigma_{CPL}}{\sqrt{N_{CPL}}}$

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where N_{CPL} and N_{CPL} are a minimum of 24 and σ_{CPL} are the 1-sigma standard deviation of the C_{PH} , C_{PL} , respectively, as defined in Section 2.4.

- 2322 For new GRUAN Ozonesonde Programmes with no launch history it is impossible to estimate
- 2323 ΔC_{PH} and ΔC_{PL} . In this case, the term shall not be used in the ozone uncertainty equation until
- after one years worth of ozonesonde launches have been processed by the GRUAN Lead Centre.
- Until such time, profiles shall be stored in CRD format until ΔC_{PH} and ΔC_{PL} can be calculated and
- then used to create the ozonesonde SGDP.

Table 6.3.1 Uncertainty estimates for the pump flow rate

	J 1 1	
ΔT_{100}	Use Equation 6.3.1	
ΔC_{PL}	Use Equation 6.3.2	
ΔC_{PH}	Use Equation 6.3.2	

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Thus, the full equation to calculate the pump flow rate uncertainty shall be expressed in the following equation

2332

2333 Equation 6.3.3 $\frac{\Delta \Phi_{P}}{\Phi_{P}} = \sqrt{\left(\frac{\Delta T_{100}}{T_{100}}\right)^{2} + \left(\Delta C_{PL}\right)^{2} + \left(\Delta C_{PH}\right)^{2}}$

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This term may change as the data record expands, thus ΔC_{PH} and ΔC_{PL} should be continually evaluated by the Ozonesonde Programmes annually to check for large deviations from its constant value and assess whether and how fluctuations in the uncertainty terms affect the ozone uncertainty significantly. It may be that re-processing of the entire data record of a given site is required if ΔC_{PH} and ΔC_{PL} statistics changes significantly over time.

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6.4 Contribution of the uncertainty in pump correction factor (PCF)

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The uncertainty in the pump correction factors (PCF), $\Delta\Psi$, shall be taken from Table 2.5.1 and are re-iterated in Table 6.4.1 below.

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Table 6.4.1 Pump correction factor uncertainties

Pressure [hPa]	Κ86 ΔΨ	Κ95 ΔΨ
Sfc-100	0.000	0.000
100	0.005	0.005
50	0.006	0.005
30	0.008	0.008
20	0.009	0.012
10	0.010	0.023
7	0.012	0.024
5	0.014	0.024

3	0.025	0.043
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Calculating $\Delta\Psi$ between data points shall be done on a log pressure scale with polynomial interpolation.

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From Table 6.4.1 the GRUAN GOASS shall use the following PCF uncertainties to the following ECC sensors:

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(i) K86 $\Delta\Psi$ for SPC ECCs

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(ii) K95 ΔΨ for ENSCI ECCs.

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New ECC sensors shall have to undergo similar JOSIE testing, laboratory and field tests to establish and validate their PCF values and uncertainties. GRUAN protocols for managing a change in sensor technology shall follow guidelines put forth in Section 7.1.

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6.5 Contribution of the uncertainty in pump temperature

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Calculating the adjusted pump temperature is discussed in detail in Section 2.6 and the associated uncertainties are summarizes in Table 6.5.1 below.

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Table 6.5.1 Uncertainties based on the location of the pump temperature thermister.

Case	Location	Sonde Type	ΔT_P	ΔT_{PCase}	ΔT_{Piston}
					internal
1	Bottom of circuit board	SPC 2A, 3A, 4A	±1.0K	±1.0K	±0.5K
2	Suspended in the styrofoam box in the vicinity of the pump	SPC 5A	±0.5K	$3.9-1.13Log_{10}(P)$ for $P > 70hPa$ $3.0-1.13Log_{10}(P)$ for $P \le 70$ hPa	±0.5K
3	Taped thermister at the pump base	SPC 5A	±0.5K	Same as Case 2	±0.5K
4	Epoxied at the pump base	SPC 5A	±0.5K	±0.5K	±0.5K
5	Mounted inside the pump body, close to the piston	EnSci Z & 2Z, SPC 6A	±0.5K	No uncertainty	±0.5K

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The additional correction to account for differences between moving piston, T_{piston} , and the internal pump, or pump based, temperatures is defined as $\Delta T_{piston-internal} = \pm 0.5 K$ and is true for all cases.

 $\begin{array}{c} 2370 \\ 2371 \end{array}$

The full contribution of the measured pump temperature to the ozone uncertainty includes the uncertainty of the additional corrections defined in Section 2.6 and summarized in Table 6.5.1.

2374 This equation is expressed as

Equation 6.5.1

$$\frac{\Delta T_{\rm P}}{T_{\rm P}} = \sqrt{\left(\frac{\Delta T_{\rm P}}{T_{\rm P}}\right)^2 + \left(\frac{\Delta T_{{\rm P}Case_i}}{T_{\rm P}}\right)^2 + \left(\frac{\Delta T_{piston-int\ ernl}}{T_{\rm P}}\right)^2}$$

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2379 6.6 Contribution of the uncertainty in the conversion efficiency

- 2380 GRUAN shall adopt the WMO/GAW uncertainty calculation for the conversion efficiency [Smit
- 2381 et al., 2014, Equation E-3-4], written as

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 $\frac{\Delta \eta_C}{\eta_C} = \sqrt{\left(\frac{\Delta \alpha_{O3}}{\alpha_{O3}}\right)^2 + \left(\frac{\Delta S_{O3:I2}}{S_{O3:I2}}\right)^2} \quad \text{where,}$ Equation 6.6.1 2383

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- 2385 $\Delta \eta_{\rm C}/\eta_{\rm C}$ = conversion efficiency uncertainty term to be used in the ozone uncertainty equation
- 2386
- 2387 $\alpha_{\rm O3}$ = absorption efficiency from the gas into liquid phase of the sensing solution = 1.0
- 2388 $\Delta \alpha_{O3} = \alpha_{O3}$ uncertainty = ± 0.01
- 2389 $S_{O3:12}$ = stoichiometry of the conversion of O_3 to I_2 = 1.0
- $\Delta S_{O3:12} = S_{O3:12}$ uncertainty = ± 0.02 at Z=0km with a linear increase to ± 0.05 at Z=35km. This 2390
- 2391 translates to the linear equation,

2392

2393 $\Delta S_{03:12}(Z) = 0.000857143*Z + 0.02$ Equation 6.6.2

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- 2395 Setting the absorption efficiency (α_{O3}) equal to one are for cases where the volume of the cathode solution is 3.0 cm³. GRUAN will use the following WMO/GAW equations to calculate α_{O3} for a 2396 2.5 cm³ volume, as follows
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Equation 6.6.3 $\alpha_{O3}(P) = 1.0044 - 4.4x10^{-5}*P$ Equation 6.6.4 $\alpha_{O3}(P) = 1.0$ 2399 100 hPa < P < 1050 hPa 2400 $P \le 100 \text{ hPa}$

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2402 $\Delta\alpha_{O3}$ is ± 0.01 for both cathode volumes.

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GRUAN shall require new candidate sites to use 3.0 cm³ volume cathode sensing solution to 2404 2405 reduce added uncertainty in the ozone uncertainty equation and maintain a constant absorption 2406 efficiency throughout the profile measurements.

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6.7 Contribution of the uncertainty in the radiosonde temperature and 2408 pressure to ozone uncertainty 2409

- 2410 The designated GRUAN Ozonesonde Lead Centre shall adopt the GRUAN Radiosonde
- 2411 Technical Report (X.X.X) processing procedures for calculating the uncertainties associated with
- 2412 the radiosonde measurements. Handling biases in the geopotential height calculation in the

- absence of GPS measurements shall be the responsibility of the Radiosonde WG-GRUAN, assigned task team, and responsible Lead Centre.

7 MANAGING CHANGES

- 2416 Changes in instrumentation, operating procedures, and data processing algorithms are likely to
- 2417 introduce sources of operational uncertainty into the ozone profiles measured within GRUAN
- 2418 Ozonesonde Programmes. The primary goals are to (i) avoid unnecessary changes, i.e. those
- 2419 changes that have no scientific, financial or operational benefit, and (ii) where changes are
- 2420 beneficial and/or necessary, to manage those changes in a way that the homogeneity of the
- 2421 ozonesonde data record is maintained across the transition and that the change does not
- 2422 compromise the integrity of the long-term record.

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- 2424 Ozonesonde have gone through several modifications since they were first introduced in the
- 2425 1960's and there is no reason to believe that those modifications will cease. Without such
- 2426 modifications there would be no opportunity to improve the performance of the instruments.
- 2427 Therefore, while GRUAN encourages ozonesonde manufacturers to improve the performance of
- 2428 the instruments, GRUAN also recognizes that managing such changes in instrument design or
- 2429 function is essential for determining long-term stability of the ozonesonde data products.
- 2430

2431 Factors influencing trends in an ozonesonde dataset to consider include the following changes 2432 (termed as "9 items" hereinafter):

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- 1. SOPs
- 2435 2. GOASS data processing algorithms
- 2436 3. ECC-sensor manufacturer
- 2437 4. Solution concentration
- 2438 5. Location of launch site
 - 6. Operating environment of the ozonesonde
- 2440 7. Ground station system
- 2441 8. Radiosonde manufacturer
- 2442 9. Including refurbished ECC-sensors

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2444 They are all likely to introduce inhomogeneities into ozonesonde SGDP. This section describes 2445 the protocols for managing changes in the ozonesonde SGDP. This section is developed based on

2446 the section "Managing change" of the GCOS-171 GRUAN Guideline.

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Guiding principles 7.1

2449 The GCOS climate monitoring principles relevant to guiding principles for managing changes in 2450 GRUAN Ozonesonde Programme include:

- 2452 The impact of new ozonesonde systems or changes to existing systems should be assessed prior to implementation. 2453
- 2454 A suitable period of overlap for new and old items is required. This will be dictated 2455 by the GCOS-171 guidelines and is addressed further in Section 7.7.

• *Embracing change*: GRUAN Ozonesonde Programmes must not be resistant to change but must actively encourage carefully managed changes. However, the advantages of making any change must always be weighed against the inherent disadvantages of making a change.

- *Change event notification*: A change event begins with the start of change of any one of the above "9 items".
 - A change event notification is first issued by the GRUAN site by email to the GRUAN Lead Centre.
 - The Lead Centre, a GRUAN Ozonesonde Programme, an ozonesonde instrument manufacturer, or another member of the GRUAN community can initiate a proposal for changes.
 - A change event ends with the official acceptance of the change that has been made after a careful and rigorous assessment. Proposed changes in (1) and (2) of the "9 items" will likely be initiated by the Lead Centre.
 - *Justification of change*: Any change to the "9 items" above in a GRUAN Ozonesonde Programme must be fully justified before the change is enacted. An assessment report must be submitted in which advantages and disadvantages of making the change must be carefully assessed. Laboratory tests of old and new items (anyone of the "9 items" listed above) should be included in the assessment report.
 - The Lead Centre must act as a clearinghouse for all proposed changes to (a) assure high stability and (b) decide when an improvement merits a change to the GRUAN ozonesonde procedures.
 - The Lead Centre, in consultation with ozonesonde experts, makes an initial evaluation of the proposed change.
 - If considered to be worth pursuing, the Lead Centre assesses the advantages, disadvantages, and potential impacts of the proposed change.
 - The information and data required to manage the change are captured in a "change evaluation report" that will become a key component of the metadata associated with the change.
 - *Preparing for change*: A quantitative assessment of the impacts of any planned change must be undertaken before the implementation of the change.
- The assessment must cover a sufficient period of time, not just covering the change period.
 - o If the knowledge needed for quantitatively assessing the impact of changes exists, it should be immediately encapsulated in the metadata associated with the change event. Official acceptance of the change should be expedited so that there is no disruption to the launch schedule.
 - Some changes have already been anticipated and assessed in this Document with a change implementation process as part of the GOASS (e.g. changing from SPC to

ENSCI, or changing solution strength (See Section 7.2)). In this case, official acceptance of the change should be expedited so that there is no disruption to the launch schedule.

- o If additional laboratory studies or dual ozonesonde launches are required, such studies must be undertaken by either the Lead Centre, a task force commissioned by the Lead Centre, the GRUAN site scientists, members of the ASOPOS panel, or other ozonesonde experts. Any relevant results in the peer-reviewed literature should be included in any change assessment.
- The impact on the ozonesonde SGDP product and its uncertainty needs to be assessed in such a way that (1) knowledge of the newly changed item is at least as detailed as knowledge of the old one, (2) tests are, or have been, conducted (e.g. processing a large number of common datasets by both new and old algorithms if a change in algorithm is proposed), (3) the resulting ozonesonde SGDP after the change are either unchanged or an improvement to those prior to change, in terms of continuity, accuracy or integrity. If continuity, accuracy and integrity cannot be improved at the same time, at least they should not be worse than before. If a considerable improvement in one aspect (e.g. accuracy) is gained, at the cost of a slight degradation of the other aspects, it might be still justifiable to propose a change.
- When laboratory studies and dual ozonesonde launches are proposed to be conducted, regular observations schedule must not be interrupted. In the case when laboratory or field studies cannot be reconciled, this must be noted as part of the metadata. In this case, a proposal of how to resolve the discrepancy should be developed by the Lead Centre WG-GRUAN.
- If the GRUAN site decides to proceed and implement the change, any data and metadata collected as part of the change process, as well as a full report on how the change is managed and implemented, must be submitted to the Lead Centre within 3 months of the completion of the change. This information will then be archived as part of the metadata record for the ozonesonde data series from that GRUAN site.
 - Validating impacts: No discontinuities in the measurement series should occur if a change has been properly managed. This is done through the justification (5) and preparing for change (6) items. Validation of the process can be achieved by subjecting the entire measurement series to homogenization tests, or may require a reprocessing of historical data. Impacts of changes must be assessed in light of the different intended uses of GRUAN ozonesonde data products.
 - Change and uncertainty: Knowledge of an ozonesonde measurement system can never be complete or perfect. Transitioning from an old to a new measurement system always introduces an additional source of uncertainty which must be captured in the uncertainty estimate on the measurements.
 - Supporting reprocessing: As new and more in-depth knowledge of ozonesonde instrumentation and processing is gained, and in particular following change events (see #4), reprocessing of historical data may be necessary. Such reprocessing may require revision of the homogenization procedures applied at each previous change

- event to produce a homogenized data record. It is essential, therefore, that raw data, as was well as detailed metadata collected during change events, are archived so that such reprocessing can be easily achieved.
 - Single changes: Whenever a measurement system is changed, as many similarities as possible between the old and new systems should be maintained e.g. both the ozonesonde and ground-station should not be simultaneously changed. Multiple simultaneous changes must be avoided so that the quantitative assessment of the impact of the change on the measurement and its uncertainty is not confounded with other, simultaneous, assessments.
 - *Monitoring changes*: Most changes are planned and therefore can be managed. However, some changes may be unplanned (e.g. natural disaster, changes in funding). Under these circumstances, GRUAN sites shall be placed on hold until the site can be re-established. It may be that re-certification is required. This shall be determined by a site visit from members of the Lead Centre (see Section 3.2).
 - *Use of independent, redundant measurements*: Redundancy in ozone measurement systems provides a powerful tool for validating the management of changes in any one of those systems. To take advantage of measurement system redundancy, it is essential that these independent systems are not changed simultaneously.
 - *Use of models*: Where changes in an historical measurement record have not been adequately managed, and where physical or statistical models can faithfully reproduce the key characteristics of the measurement record, the model time series can provide a means of detecting and correcting for systematic biases between old and new measurement systems. In GRUAN, where all changes are managed changes, the use of models for this purpose should not be necessary.
 - Manufacturer involvement: Efforts must be undertaken to avoid unknown changes
 e.g. the instrument manufacturer making unannounced changes. GRUAN needs to
 establish close working relationships with instrument manufacturers so that any
 changes implemented in the manufacturing of an instrument are made know to the
 GRUAN ozonesonde community.

7.2 Transfer Functions

- There have been a number of studies that have used laboratory, dual-sonde, and multi-sonde payloads to derive methods of calculating transfer functions that characterize differences in instrument and solution concentration [Smit et al., 2007; Kivi et al., 2007; Deshler et al., 2008; Stu bi et al., 2008; Mercer et al., 2008].
- As part of the SPARC-IGACO-IOC-NDACC (SI2N) initiative, the Assessment of Standard Operating Procedures for Ozone Sondes (ASOPOS) working group established empirical transfer functions specifically for the SPC and ENSCI type ozonesondes using either the 1% full buffer or 0.5% half buffer solutions [Smit et al., 2012]. This work uses all data taken from the above cited studies. Their aim is to homogenize long term ozonesonde records, that use these

sensor/solution combinations, for ozone assessments of changes in the vertical distribution of ozone [http://igaco-o3.fmi.fi/VDO/documents.html]. 2579

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These transfer functions represent the quantitative differences of the ozonesonde response based on changes in instrumentation and stoichiometry of the conversion of O₃ to I₂ with a change in solution concentration. They are not a reflection of changes in SOPs. Smit et al. [2007] and Thompson et al. [2007] showed that there are discontinuities in the time series of a single site that have used a variety of instruments and solution strength, citing the need to homogenize the long term records of individual ozonesonde sites.

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The conversion relationship is summarized in Table 3 of Smit et al. [2012].

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GRUAN processing protocol

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- 1. Where applicable, transfer functions taken from Smit et al. [2012] shall be applied and shall be part of the ozonesonde SGDP.
- 2594 2. Data records where transfer functions should be applied but do not yet exist shall remain 2595 in the Level 2 stage but shall not be considered as part of the ozonesonde SGDP.
 - 3. Transfer functions for time series that use a combination of BM and ECC shall follow WMO/GAW #201 Report guidelines found in Section 4.3 and subsections. It shall be the responsibility of the Lead Centre and the WG-GRUAN to evaluate the appropriateness of the transfer functions and determine if BM data records are of sufficient quality to meet the GRUAN reference measurement standards.
 - 4. As of this document, there are no transfer functions for time series that use a combination of CI and ECC sondes. However, dual sonde launches have been conducted by Nakamura et al., [2008] and have the potiential to be used to develop transfer functions. The Lead Centre and WG-GRUAN shall work with the manufacturer (Japanese Meteorological Agency) to determine the extent to which uncertainties estimates have been established and validated and the status of deriving transfer functions between CI and ECC sondes by the group. It shall be the responsibility of the Lead Centre and the WG-GRUAN to evaluate the appropriateness of the transfer functions and determine if the historic CI data records are of sufficient quality to meet the GRUAN reference measurement standards.

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7.3 Managing changes in instrumentation

- 2612 GRUAN Ozonesonde Programme is characterized by the fact that every ozone profile is 2613 measured with a different instrument. Managing changes in instrumentation therefore extends to
- 2614 managing changes in sondes between flights. Efforts must be undertaken to avoid unknown
- 2615 changes e.g. the instrument manufacturer making unannounced changes to the material or
- configuration of the ECC sensor, or a ground station software update. Late response to changes 2616
- 2617 or upgrade announcements may result in discrepancies in the measurement time series. One way
- 2618 to ensure that instrument changes are identified, characterized, and recorded such that there is no
- 2619 discontinuity in the network, as a whole, is for mandatory GRUAN representation at future

JOSIE studies. This will not only safeguard the homogeneity of datasets due to instrumentation changes but will also ensure that GRUAN:

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- Follows retractions or addendum's to the original GAW Report No. 201
 recommendations and SOP protocols.
 - 2. Be informed of changes in manufacturer design and materials, and how these affect ozonesonde performance.
 - 3. Be aware of changes in the processing software.
 - 4. Be advised of additional concerns in the SOPs.

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All of the above will impact GRUAN processing procedures. Therefore, GRUAN participation should be mandatory.

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2633 GRUAN Lead Centre needs to establish close working relationships with ozonesonde instrument manufacturers (e.g. SPC and ENSCI) and ozonesonde/radiosonde ground station manufacturers 2634 (e.g. Vaisala, Modem, Chang Feng, etc) so that any changes to be implemented or having been 2635 implemented are known to them. Preferably the changes can be known substantially in advance 2636 of deployment, allowing sufficient time to investigate, understand, prepare for and document the 2637 2638 change and its likely impacts. Links to instrument manufacturers: Dealing with changes in 2639 instrumentation will require GRUAN task team to establish close two-way links to instrument 2640 and ground station manufacturers. Inclusion of ASOPOS panel members, other ozonesonde experts, and other ozonesonde archives (e.g. SHADOZ and NDACC) in discussions of 2641

instrument change would be advantageous.

of the long-term practices.

7.4 Managing changes in SOP and operating environment

2644 Currently, there are multiple variations in ozonesonde preparation procedures since the first 2645 manual was written [Komhyr, 1986]. Besides modifications in the manufacturer's instructions in 2646 past the decades, scientific institutions have established their own modified operating 2647 procedures. There is also a number of ozonesonde processing software that applies their own 2648 treatment of the variables that go into Equation 1. Testing of the ozonesondes under laboratory 2649 conditions has showed the need to standardize the operating procedures and provide guidelines 2650 to homogenize the data based on community consensus [Smit et al., 2014]. Smit et al., [2007] 2651 reports that maintaining SOPs improves the precision of the overall measurements better than 2652 ±3-5%. GRUAN recommends that each station maintain the GRUAN Lead Centre certified set 2653 SOPs for pre-flight and day of flight conditioning established by WMO/GAW to ensure 2654 consistency and homogeneity in operating practices. The goal here is not to disrupt the continuity

- As described in Section 3.5, while implementing these SOPs is not mandatory, sites are required to document where they have deviated from the GRUAN certified SOPs and, when audited, are assessed for their ability and willingness to adhere to the SOPs within GRUAN.
- Some changes in the operating environment may be unplanned, such as in the event of a natural disaster, erosion of the field site or land-use changes that necessitates moving the operating
- environment. Under these circumstances, a GRUAN site shall be placed on hold until the

- 2663 physical site can be re-established. It may be that the new location is far enough away from the
- original location that a new GRUAN site needs to be established in place of the old site. This
- shall be determined by the task team assigned by the Lead Centre. In this case, re-certification
- will be required because the new location and operating conditions will need to be re-assessed.
- 2667 The process of re-certification shall follow the guidelines addressed in Section 3.2.
- 2668 In their annual report, each site shall document any changes to their current certified SOPs and
- operating environment and include (1) why those changes occurred, (2) how those changes were
- 2670 managed, and (3) the impact, if any, on the homogeneity, accuracy, and integrity of their
- measurements.

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GRUAN sites shall follow the change protocol outlined in Section 7.1 if changes to items (1) and (6) of the "9 items" occur.

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- 2676 GRUAN representation at future JOSIE studies is strongly recommended to follow (1)
- retractions or addendum's to the original WMO/GAW Report No. 201, (2) recommendations and
- SOP protocols, and (3) be advised of additional concerns in the SOPs.

2679 7.5 Managing changes in data processing algorithms

- As in any data processing situation, there will be occasional re-processing of the ozonesonde
- 2681 converted raw data (CRD) after updates/upgrades of the GRUAN GOASS, addressed in Section
- 2682 3.7. The GOASS must be transparent, i.e., developed and optimized in consultation with WG-
- 2683 GRUAN members. WG-GRUAN shall meet regularly to discuss the implementation of updates
- 2684 to the GOASS, whether they pertain to one site or the entire ozonesonde network. Planned
- 2685 changes in data processing algorithms should be dealt with in a fashion similar to planned
- 2686 changes in SOPs (Section 7.4).

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- Changes in the GOASS may be due to the following:
 - 1. New or modified transfer functions (Section 7.2)
 - 2. Updated uncertainty calculations (Section 6)
 - 3. Changes in the pump efficiency factors (Section 2.5)
 - 4. Changes in the partial ozone column calculation above balloon burst (Section 2.7)
 - 5. Changes in the Metadata (Section 3.6)

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Changes resulting in (2) – (5) will likely result in the complete reprocessing of entire data sets across the network. Since there is a time and administrative cost associated with the reprocessing of a record, such reprocessing should only be undertaken when justified. Protocols must be established by the designated Lead Centre ozonesonde data processing facility to indicate when reprocessing of the full measurement record at any site is justified or required.

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Traceability is a leading component of GRUAN. Every single GOASS update must be associated with an increment of the data processing version. A system of traceable version numbers for all ozonesonde level products has been developed to allow for a full identification and tracking of the data processing changes made since the initial product delivery. This product versioning system shall be determined by the Lead Centre task team.

Data processing updates must be communicated to users who have accessed earlier versions of the data and who have voluntarily registered to receive notifications of such data updates (see Section 8.6 of the GRUAN Guide). Therefore, all older product versions must be made available through the GRUAN archives.

2712 7.6 Managing changes in calibration

- When ozonesondes are calibrated to fundamental calibration standards as part of the pre-flight
- 2714 ground-check, changes in sonde performance can be more easily managed. If possible, the
- 2715 impacts of a change in calibration should be quantified through traceability of the calibration
- 2716 standard. For example, the WCFOS in JOSIE studies satisfies the protocols for maintaining
- 2717 ozonesonde continuity, accuracy and integrity threw periodic quality checks of instrumental
- 2718 performance of ozonesonde from different manufacturers, and establishing up-to-date SOPs.
- 2719 It would ideal to establish guidelines by which a GRUAN Ozonesonde Programme can calibrate
- 2720 its ground station equipment such that sources of error and uncertainty can be further identified,
- traced, and included as part of the uncertainty budget for ozonesondes. Metadata provides a
- traceable source from which a change in the essential characteristics of each unique ozonesonde
- sensor can be identified, measured, and recorded (essential metadata are addressed in Section
- 2724 3.6).

7.7 Validating changes using parallel observations

Cases where parallel observations are applicable to the ozonesonde programme are the following (hereafter called "4 cases"):

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- A new ECC sensor is developed
- A new sensing solution recipe is developed
- Change in SOPs
 - Change in radiosonde manufacturer and/or model

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2734 If any of the above changes occur, a combination of JOSIE studies, other laboratory inter-

2735 comparisons, and dual sonde launches must be made to establish (1) new precision and accuracy

estimates, if any, (2) changes in uncertainties, and (3) new transfer functions to maintain

2737 homogeneity within a time series of a single site and within the network. While these studies are

proposed and conducted, the regular observations schedule must not be interrupted. In the case

when laboratory studies cannot be reconciled, this must be noted as part of the metadata. In this

case, a proposal of how to resolve the discrepancy should be developed by the Lead Centre or a

task force commissioned by the Lead Centre.

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- 2743 *Measurement redundancy*: Measurement redundancy (see Section 6.2 of GCOS-171) highlights the benefits for managing instrumentation change. If parallel observations of the above four
- changes are not feasible, the availability of additional redundant measurements with similar
- 2746 sampling attributes (vertical resolution, temporal sampling frequency etc.) is essential for
- validating a managed change. In such cases, an evaluation of the redundant system(s) with the
- old and new systems over an overlap period of at least 12-months must be undertaken to validate
- the robustness of change management.

- 2751 *Inter-comparisons*: Formal measurement inter-comparisons, in the form of dual ozonesonde
- 2752 launches are essential for developing the in depth understanding required to manage changes in
- 2753 the "four cases". For this reason, participation in inter-comparisons is expected. Outcomes from

- 2754 such inter-comparisons must form an important component of the metadata archived at the
- 2755 GRUAN Lead Centre. GRUAN Ozonesonde Programme should participate in, or leverage from
- 2756 WMO and partner networks (e.g. SHADOZ and NDACC) instrument inter-comparison
- 2757 campaigns.

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7.8 Implementation of Network-wide changes

- 2760 Considering the critical importance of change management and that GRUAN sites must not act
- 2761 unilaterally in implementing changes, a procedure for implementing network-wide changes has
- been described in Section 2.3.11 of the GRUAN Guide to Operations.
- 2763 Managing change is essential to maintaining network homogeneity. Changes in ozonesonde
- 2764 measurement systems, i.e. the "9 items", at GRUAN sites should therefore be conducted in such
- a way that the homogeneity of the resultant GRUAN ozone data products across the network is
- 2766 not compromised. The Lead Centre shall play a key role in ensuring such smooth transitions. In
- 2767 particular changes in (1) and (2) of the "9 items" will require network-side changes to ensure
- homogeneity.

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- 2770 The Lead Centre should consult with ozonesonde experts (e.g. members of the ASOPOS panel),
- science experts from the four key user communities, and other ozonesonde archive centres such
- as SHADOZ and NDACC to thoroughly evaluate the potential implications of network wide
- implementation of the proposed change. If the proposed change is approved, the Lead Centre, in
- 2774 consultation with the nominated central processing facility, will develop a formal change plan for
- implementation across the network. The formal change plan is then communicated to all
- 2776 GRUAN ozonesonde sites within the network. Any changes or deviations from the documented
- 2777 approvals must be considered a new change and must be reassessed by the Lead Centre.

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- However, changes are not necessarily always network-wide. In some circumstances, changes to
- an individual site are allowed which do not compromise network homogeneity, for instance
- changes in instrument or solution concentration, a change in instrument operators, or change of
- operating environment. Documentation of these site changes in the form of metadata is essential.
- 2783 Sites will be audited on the completeness of their metadata submitted to GRUAN archives as
- 2784 part of the site assessment and certification process. Also see #9 in Section 7.1 Supporting
- 2785 reprocessing.

7.9 Data and metadata traceability

- 2787 It is essential that metadata associated with the site and each ozonesonde instrument launched,
- 2788 and in particular change events (see Section 7.1) that may cause discontinuities in the
- 2789 measurement time series, are captured. Sufficient metadata must be available to tie the new
- 2790 SGDP via a comparable traceability chain, back to the same recognized standard as the old
- 2791 SGDP.

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- 2793 Storage: It is essential that a secondary back-up storage of raw data (L0 PRD) be maintained at
- each GRUAN site. Metadata on written on check lists should be digitized and stored similarly
- with the raw data. Each sites data storage policy shall be evaluated by the WG-GRUAN as part
- of the site assessment and certification process (Section 3.2), and re-evaluated in audits and
- annual reports.

Launch scheduling: Measurement scheduling shall remain stable unless there is a clear
 requirement for change. Amendments to the GRUAN measurement scheduling protocol shall be
 submitted by the WG-GRUAN before being distributed to GRUAN sites for implementation. In
 recognition of the heterogeneity of the network, the scheduling protocols defined in this
 Document may not apply at every GRUAN site, but any deviation from the measurement
 schedule must be agreed by the GRUAN Lead centre and then accepted by WG-GRUAN.

 Metadata changes from the GRUAN check list: As described in Section 3.6, while using the GRUAN check list is not mandatory, sites are required to document where they have deviated from the prescribed check list and, when audited, are assessed for their ability and willingness to adhere to them within GRUAN.

Importance of Metadata: Metadata is a critical component when documenting network changes. Complete metadata should include a full account of the ozonesonde operation from the time the sensor is taken out of its' box to the time of launch release. Detailed archiving of instrument metadata will be vital to managing changes in instrumentation. This will allow later reprocessing of the raw data as thoroughly as possible (see Section 2.3.4 of GCOS-171). A detailed description of how each change in a measurement system was managed can be found in the GRUAN check list (Appendix A-1) and a complete list of the essential metadata components is in Section 3.6. These metadata lists include everything related to the quantitative assessment of the impact of the change on the measurement and its uncertainty.

8 QUALITY MANAGEMENT 2822

- 2823 This section defines the principles and the methodological framework for GRUAN operations,
- 2824 and details how activities will be coordinated to manage and control data quality within
- 2825 GRUAN. This section draws heavily from Section 10 of GCOS-171 and reiterates much of the
- 2826 data management policies central to all GRUAN measurement programmes.

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2828 Quality management within GRUAN consists of quality assurance and quality control:

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2830 *Quality assurance* (QA): The purpose of quality assurance is to provide confidence that the requirements for achieving quality will be fulfilled. QA includes all the planned and systematic 2831 2832 activities that will be implemented such that quality requirements for a product or service will be

2833 fulfilled.

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Quality control (QC): The purpose of quality control is to ensure that the expectations created by QA are fulfilled. QC is associated with those operational methods, techniques and activities used to ensure that the quality requirements (as defined by QA) are fulfilled.

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The GRUAN quality management policy is to achieve a level of data quality that allows the primary goals of GRUAN to be met for all potential users of GRUAN data products. Quality assurance i.e. implementing systems to ensure quality, and quality control i.e. monitoring the results to ensure that the systems implemented are adequate to the task, are both required at all stages of the GRUAN ozonesonde data production. Because GRUAN ozonesonde data products are intended to be used for long-term trend detection, quality assurance and control are further extended to data re-processing and to the management of long-term consistency and stability (addressed in Section 7 of this Document).

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Methods by which QA for Ozonesonde Programmes can be achieve is through the following:

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1. The use of redundant measurements, as described in Section 4.1.2, serves to assure the quality of the GRUAN data products. Agreement of two independent measurements (e.g. Lidar and Microwave Radiometer), preferably based on different measurement principles, provides a high degree of confidence that no significant systematic effect was disregarded and uncertainties were not under-estimated.

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2. Laboratory tests are fundamental methods for establishing and confirming uncertainty estimates and transfer functions for GRUAN data products. Laboratory tests provide an opportunity to investigate in detail the performance of instruments under controlled conditions and to measure differences against certified references or other standards (e.g. JOSIE). Data from these experiments can be used to detect biases that may be corrected for and to determine calibration uncertainties.

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2865 2866 3. Field inter-comparisons (dual or multi sonde launches on a single payload) allow multiple in-situ sensors to be directly compared under the actual atmospheric conditions of the required measurement, including the complex environmental conditions (temperature, humidity, pressure, wind/flow rate, radiation, and chemical composition) that cannot be fully reproduced in the laboratory. These complementary activities increase confidence

that measurements are subject to neither unanticipated effects nor undiscovered systematic uncertainties. Therefore field experiments are particularly useful for assuring the quality of GRUAN data products.

QC will be achieved through the application of the various measurement protocols defined in this Document and in related measurement system documents (e.g. Lidar, Radiosonde technical documents). To the extent possible, visual inspection of all data by science/instrument experts will be required for ozonesondes to minimize anomalies that slip through automated routines. The Lead Centre shall coordinate this effort, which shall be distributed across different GRUAN sites and other interested parties as deemed appropriate including task teams and members of WG-GRUAN. Vertically resolved uncertainty estimates, calculated by the GOASS for each site, will be used as a metric to compare the site-to-site quality of the observations.

Quality management is required at all points in the measurement process from network planning and training, through installation and site operations to data transmission and archiving. This quality management must include feedback and follow-up provisions across a range of timescales from sonde conditioning to annual reviews. Because of the emphasis on the provision of robust measurement uncertainties and the associated requirement for in-depth quality management, the resources required within GRUAN to undertake quality management will likely be a significant proportion of the cost of operating the network, and very likely more than the few percent of overall operating costs typical of many observational networks. However, without this expenditure, the quality of the data will be unknown, and their usefulness diminished.

A key aspect of quality management within GRUAN will be fulfilling customer requirements. To this end systems shall be developed to:

- 1. Inform users of GRUAN products of changes in measurements systems at specific sites.
- 2. Provide an incident reporting system that can flag data anomalies to users.
- 3. Inform users of the availability of updates to previously accessed data products.
- 4. Provide "help desk" support to users of GRUAN data products.
 - 5. Establishing close working relationships with instrument manufacturers will also be central to quality assurance within GRUAN.

8.1 Assuring the quality of GRUAN Ozonesonde Programmes

The purpose of quality management is to ensure that GRUAN data meet the requirements in terms of uncertainty, resolution, continuity, homogeneity, representativeness, timeliness, format etc. for their intended use, at a minimum practicable cost. GRUAN recognizes that all measurements are imperfect, but, if their quality is known and demonstrable, they can be used appropriately. Minimizing cost without compromising quality is also an implied or explicit requirement for measurements made within GRUAN.

Five critical components are required to assure the long-term quality of GRUAN Ozonesonde Programmes include:

- 2910 1. Maintaining consistent, up-to-date SOPs to minimize systematic errors and lend confidence in the observed trends.
 - 2. GRUAN-specific training of the representative and ozonesonde technicians of candidate ozonesonde sites, the purpose of which is to ensure that the latest GRUAN-recommended best practices for ozonesonde operations are observed.
 - 3. The RSLaunchClient utility, the purpose of which is to upload, the raw measurement data and metadata to the GRUAN central ozonesonde data processing facility.
 - 4. The GOASS, the purpose of which is to analyses in a consistent manner the converted raw ozonesonde data (CRD) through the RSLaunchClient, and to calculate the ozonesonde SGDP and their uncertainties.
 - 5. Maintaining documentation and statistics on flagged metadata (addressed in Section 3.7), and missing raw data to be used as a diagnostic tool as part of the quality control assessment and to ensure the continuity of individual GRUAN Ozonesonde Programmes.

Routine testing of newly manufactured ozonesondes, changes in instrument design or solution recipes will help to ensure confidence in observed trends in the future. Therefore, as part of the quality assurance (QA) for ozonesondes that are in routine use, GRUAN shall follow protocols established by the Forschungszentrum Jülich which houses the World Calibration Center for Ozone Sondes (WCCOS) [http://www.fz-juelich.de/iek/iek-

8/EN/Expertise/Infrastructure/WCCOS/WCCOS.html?nn=865134]. The simulation facility enables control of pressure, temperature and ozone concentration and can simulate flight conditions of ozone soundings up to an altitude of 35 km, whereby a UV photometer serves as a reference [Smit et al., 1998]. The long term objective of WCCOS is to ensure thee major QA-tasks:

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- 1. QA-Procedures: Establishment and up-date of SOPs of different sonde types.
- 2. QA-Manufacturers: Performance check of ozonesondes from different manufacturers
- 3. QA-Operation: Evaluation of ozonesonde operating practice of difference sounding laboratories

8.2 Raw data validation

Quality control at the raw data level is performed in two steps, first through uploads of the most recently acquired raw data and associated metadata through the RSLaunchClient utility, then through the threshold quality checks at the early processing stage of the GOASS (selection criteria are addressed in Table 3.7.1 of Section 3.7). The suitability check of the raw data and metadata to be accepted as part of the GOASS processed stream serves as a means to verify the completeness of the information required by the RSLaunchClient.

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8.3 Ozonesonde data product validation

- 2948 Ozone profiles derived from GRUAN Ozonesonde Programmes will, in the first instance, be
- 2949 validated against available redundant ozone profile measurements made at GRUAN sites (refer
- 2950 to Section 4.1.2). Multiple measurements of ozone will be invaluable for identifying,
- 2951 understanding and reducing systematic effects in ozonesonde measurements. One important
- 2952 factor for GRUAN is that redundant measurements of the same (or related) variables should be

2953 reported in a consistent way. The cross-checking of redundant measurements for consistency 2954 should be an essential part of the GRUAN quality assurance procedures. Since all data are to be reported with uncertainties, a consistency check should, in principle, be a straight forward task. 2955

2957 Satellite-based measurements of total column ozone (e.g. OMI, GOME-2) and profiles of ozone 2958 in the lower stratosphere (e.g. Aura/MLS) are common reference measurements that can be used 2959 to assess the quality of ozonesonde observations. GRUAN shall, where practical, schedule 2960 ozonesonde launches in near real-time (i.e. within 2 hours of a satellite overpass) to fulfill the requirement of providing a reference to satellite measurements. 2961

In addition, GRUAN Ozonesonde Programmes are encouraged to participate in field campaigns

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involving non-GRUAN instruments. All comparisons should be made between measurements 2968

independent from each other. If two measurements are known to be dependent, the degree of this dependence as well as its consequences must be specifically described and taken into account in

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the product assessment. As stated in Section 10 of the GCOS-171, "Agreement of two 2971 independent measurements, preferably based on different measurement principles, provides a

2972 high degree of confidence that no significant systematic effect was disregarded and uncertainties

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were not underestimated". 2974

8.4 Performance monitoring system

- 2975 Applying the principles described in Section 10 of the GCOS-171 to GRUAN Ozonesonde
- 2976 Programmes, performance monitoring is a non-real-time activity in which the performance of an
- individual GRUAN Ozonesonde Programme, or of an ensemble of GRUAN Ozonesonde 2977
- 2978 Programmes, is examined for trends and systematic deficiencies. Performance monitoring within

Certification and re-certification of GRUAN Ozonesonde Programmes is an essential component

2979 GRUAN Ozonesonde Programmes is primarily the responsibility of the Lead Centre and the 2980 TTS.

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- 2985 Ozonesonde SGDP downloads 1.
- 2986 Number of candidate sites wishing to become a GRUAN Ozonesonde Programme. 2.

of performance monitoring. Examples of quantitative performance indicators are:

- 2987 Number of GRUAN sites participating in JOSIE and inter-comparison field campaigns, 3. 2988 and conducting laboratory studies whose results appear in peer reviewed journals.
- 2989 4. The number of peer reviewed publications in which GRUAN ozonesonde data products 2990 have been used.
- 2991 5. The number of GRUAN Ozonesonde Programmes funded through national or 2992 international funding agencies.

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All above indicators serve to provide a year-to-year traceability of GRUAN ozonesonde programmes' impact within the climate community.

2997 ACRONYMS

- 2998 ASOPOS: Assessment of Standard Operating Procedures for Ozone Sondes
- 2999 BESOS: Balloon Experiment on Standards for Ozone Sondes
- 3000 CRD: Converted Raw Data
- 3001 *DMT*: Droplet Measurement Technologies
- 3002 ECC: Electrochemical concentration cell
- 3003 *ECV*: Essential Climate Variable
- 3004 *GATNDOR*: GRUAN Analysis Team for Network Design and Operations Research
- 3005 GAW: Global Atmosphere Watch
- 3006 GCOS: Global Climate Observing System
- 3007 GOASS: Ozonesonde Analysis Software System
- 3008 GOME-2: Global Ozone Monitoring Experiment–2
- 3009 GPS: Global Positioning System
- 3010 GRUAN: GCOS reference upper-air network
- 3011 *IGACO*: Integrated Global Atmospheric Chemistry Observations
- 3012 IGPD: Integrated GRUAN Product Data
- 3013 *IOC*: Intergovernmental Oceanographic Commission
- 3014 JOSIE: Jülich Ozone Sonde Inter-comparison Experiment
- 3015 *LMS*: Lockheed Martin Sippican
- 3016 NDACC: Network for the Detection of Atmospheric Composition Change
- 3017 NCAR: National Center for Atmospheric Research
- 3018 NCEI: National Centers for Environmental Information
- 3019 *NMI*: National Metrological Institute
- 3020 NOAA: National Oceanic and Atmospheric Administration
- 3021 *OMI*: Ozone Monitoring Instrument
- 3022 *PCF*: Pump correction factors
- 3023 PRD: Primary Raw Data
- 3024 SAG: Science Advisory Group
- 3025 SASBE: site atmospheric state best estimates
- 3026 SGPD: Standard GRUAN Product Data
- 3027 SHADOZ: Southern Hemisphere ADditional OZonesondes
- 3028 SPARC: Stratosphere-troposphere Processes And their Role in Climate
- 3029 SPC: Science Pump Corporation
- 3030 Suomi-NPP: Suomi National Polar-orbiting Partnership
- 3031 *TEI*: Thermo Environmental Instruments
- 3032 TTS: Task Team on Sondes
- 3033 *UTLS*: Upper Troposphere Lower Stratosphere
- 3034 WCCOS: World Calibration Center for Ozone Sondes
- 3035 WG-GRUAN: Working Group on GRUAN
- 3036 WIGOS: WMO Integrated Global Observing Systems
- 3037 WMO: World Meteorological Organization
- 3038 WOUDC: World Ozone and Ultraviolet Data Centre

Appendix A.1: GRUAN STANDARD OPERATING 3039 PROCEDURES CHECK LIST 3040 3041 Follows the WMO GAW Report #201 SOPs 3042 INITIAL PREPARATION - NO LESS THAN 3 DAYS BEFORE FLIGHT. 3043 OPERATOR INITIALS: ____ 3044 3045 FLT# DATE (YYYYMMDD): 3046 O₃ PUMP SERIAL #: 3047 3048 1. Run 10 minutes on <u>no</u> O₃ air: ____ ($\sqrt{}$) 3049 2. PUMP CURRENT: _____(μA) 3050 3. PUMP PRESSURE: _____ (psi) 3051 4. PUMP VACUUM: _____ (in Hg) 3052 5. Run 30 minutes on \underline{HIGH} O₃: $(\sqrt{)}$ 3053 6. Run 5 minutes on <u>no</u> O₃: $(\sqrt{})$ 3054 7. ADD 3.0 CC FRESH CATHODE (Wait 2 min): $\sqrt{}$ 3055 3056 8. ADD 1.5 CC ANODE SOLUTION: 9. Run 10 minutes on <u>no</u> O₃: ____ ($\sqrt{}$) 3057 10. RECORD O₃ CURRENT: μA 3058 11. Run 5 minutes at $5\mu A$ O₃ ____ ($\sqrt{}$) - then switch to \underline{no} O₃ air. 3059 12. RECORD TIME TO DROP FROM 4 TO 1.5 μA: sec. 3060 13. Run 10 minutes on \underline{no} O₃: $(\sqrt{})$ 3061 14. RECORD O₃ CURRENT: uA 3062 For refurbished sensors, follow calibration procedures. 3063 15. Add additional 2.5 cc of CATHODE : $(\sqrt{})$ 3064 3065 16. Short the cell leads: $(\sqrt{})$ 17. Intake tube stored in sonde frame: $(\sqrt{})$ 3066 18. Store inside Styrofoam flight box: $(\sqrt{})$ 3067 3068 3069 IF DORMANT AFTER 1 WEEK REPLACE SOLUTIONS. 3070 DATE (YYYYMMDD) : _____ 3071 3072 1. CHANGE CATHODE SOLUTION (3cc): $(\sqrt{})$ 3073 2. CHANGE ANODE SOLUTION (1.5cc): $(\sqrt{})$ 3. Run 5 minutes on <u>no</u> O₃ ____ ($\sqrt{}$) 3074 4. RECORD O₃ CURRENT: μA 5. Run 5 minutes on $5\mu A$ O₃ $\sqrt{\langle \psi \rangle}$ 3075 3076 6. Switch to no O_3 : $(\sqrt{})$ 3077

7. RECORD TIME TO DROP FROM 4 TO 1.5 μ A: _____ sec

8. Run 10 minutes on <u>no</u> O₃ – RECORD CURRENT: ____ uA

9. Short cell leads and Store in Styrofoam flight: $(\sqrt{})$

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3081	IF DORMANT AFTER ANOTHER WEEKS REPLACE SOLUTIONS.
3082	DATE (YYYYMMDD) :
3083	
3084	1. CHANGE CATHODE SOLUTION (3cc): ($$)
3085	2. CHANGE ANODE SOLUTION (1.5cc): $()$
3086	3. Run 5 minutes on \underline{no} O ₃ ($$)
3087	4. RECORD O ₃ CURRENT: μA
3088	4. RECORD O ₃ CURRENT: μA 5. Run 5 minutes on $5\mu A$ O ₃ $\sqrt{\langle v \rangle}$
3089	
3090	
3091	8. Run 10 minutes on <u>no</u> O ₃ – RECORD CURRENT: uA
3092	9. Short cell leads and Store in Styrofoam flight: $()$
3093	, <u> </u>
3094	DAY OF FLIGHT PREPARATION IN LAB:
3095	DATE (YYYYMMDD):
3096	OPERATOR INITIALS:
3097	
3098	1. CHANGE CATHODE SOLUTION (3cc): $()$
3099	2 CHANGE ANODE SOLUTION (1.5cc): $()$
3100	3 Run 10 minutes on no O_3 : $()$
3101	3. Run 10 minutes on \underline{no} O ₃ : ($$) 5. RECORD O ₃ CURRENT: $\underline{BG\#0} = \underline{\qquad}$ μA
3102	6. Run 10 minutes at $5\mu A$ O_3 :($$)
3103	7. Switch to <u>no</u> O ₃ :($$)
3104	8. RECORD CURRENT AFTER 30 SecμA, 1minμA, 2minμA
3105	3min μA, 5min μA, 10min μΑ
3106	pr. 1, 0 mm pr. 1, 1 mm pr. 1
3107	9. RECORD O ₃ CURRENT: $\underline{BG\#1} = \underline{\hspace{1cm}} \mu A$
3108	10. ROOM TEMP (C):, ROOM RH (%):,
3109	ROOM Pressure (hPa)
3110	
	FLOWRATE #1: sec
3112	FLOWRATE #1: sec
3113	FLOWRATE #1: sec
3114	FLOWRATE #1: sec
3115	FLOWRATE #1: sec FLOWRATE #1: sec
3116	AVERAGE T100: sec
3117	
3118	DAY OF FLIGHT AT THE LAUNCH SITE:
3119	
3120	FLT #:OPERATOR INITIALS:
3121	
3122	Dobson (if available):(DU)
3123	Brewer (if available):(DU)
3124	Other (if available):(DU)
3125	
	RADIOSONDE SERIAL #:

3127	INTERFACE # (if applicable):	
3128	O ₃ BACKGROUND CURRENT BEFORE FLIGHT <u>BG#2</u> : μA	
3129		
3130	GMT Date (YYYYMMDD):	
3131	GMT Launch Time (HH:MM:SS):	
3132	LOCAL date (YYYYMMDD):	
3133	LOCAL Launch time (HH:MM:SS):	
3134		
3135	BALLOON SIZE:Grams:	
3136	TYPE: TOTEX Hwoyee PAWAN ($\sqrt{\text{one}}$)	
3137		
3138		(m/s)
3139	SURFACE TEMP:(C) SURFACE WIND DIR:	(deg)
3140	SURFACE RH: (%)	
3141	Sky Conditions and General Remarks:	
3142		
3143		
3144		

Appendix A.2: RECOVERED OZONESONDE CHECKLIST Follows the NOAA/ESRL/GMD Check list DATE (YYYYMMD): _____OPERATOR INITIALS: _____ Was this a GPS Sonde recovered on day of flight? ____ Yes/No If No, how many days between launch and recovery? days **HISTORY**: O₃ PUMP SERIAL #: _____ FORMER FLIGHT #: DATE FLOWN (YYYYMMDD): _____ DATE FOUND (YYYYMMDD): _____ DATE RETURNED (YYYYMMDD): **COMMENTS:** OVERALL SONDE/PUMP CONDITION: (looks new, dirt or coloring around pump present, signs of corrosion anywhere, 0-ring condition, pump noisy?, etc.) INITIAL RINSE/RECONDITIONING – SOON AFTER DELIVERY: Check that the cam that drives the piston is not turning off-center, loose or rubbing too close to the metal frame. If it is too close or has come loose then the sonde will be noisy and run with a high current. Sonde should not be flown in this case. Rinse off outside of cells with warm tap water. $(\sqrt{})$ Squirt De-ionized water (DIW) through running pump inlet (2 or 3 times for about 5 seconds). ___(\sqrt{) Rinse cells and tubing with DIW. ____($\sqrt{}$) Fill cells about $\frac{3}{4}$ full of DIW. ($\sqrt{}$) Store sheet and ozonesonde until ready for the 3-7 day pre-condition. $(\sqrt{})$ Date stored on shelf until ready for the 3-7 day pre-condition (YYYYMMDD):

3186 3187 3188	During normal pre-conditioning preparations , an ozone calibrator, e.g. TEI, is strongly recommended to test the performance of the refurbished sonde. Re-conditioned sondes should not be flown if the sonde values are $\pm 5\%$ of calibrated source.
3189	
3190	PRE-CONDITIONING CALIBRATION PROCEDURES:
3191	
3192	DATE (YYYYMMDD):
3193 3194	Operator Initials:
3195	Calibration Instrument/Model:
3196	Calibration Serial Number:
3197	
3198	1. Run 50 ppbv O_3 for 10 minutes: ($$)
3199	2. Record: CALIBRATOR: ppbv OZONESONDE: ppbv % Difference:
3200	3. Run 100 ppbv O_3 for 10 minutes: ($$)
3201 3202	4. Record: CALIBRATOR:ppbv OZONESONDE:ppbv % Difference:
	5 Pure 150 males O. for 10 minutes:
3203	5. Run 150 ppbv O_3 for 10 minutes: ($$)
3204 3205	6. Record: CALIBRATOR: ppbv OZONESONDE: ppbv % Difference:
3206	7. Run 200 ppbv O_3 for 10 minutes: ($$)
3207	8. Record: CALIBRATOR:ppbv OZONESONDE:ppbv % Difference:
3208	9. Run 50 ppbv O_3 for 10 minutes: ($$)
3209	10. Record: CALIBRATOR:ppbv OZONESONDE:ppbv % Difference:
3210	
3211	11. Run <u>no</u> ozone air for 10 minutes: ($$)
3212	12. Record: CALIBRATOR: ppbv OZONESONDE:ppbv % Difference:
3213	
3214	IC 41
3215	If the percentage differences for the 100 ppbv and ozone-free air exceeds $\pm 5\%$ do not fly re-used sonde.
3217	Solide.
3218	
3219	FINAL COMMENTS:
3220	
3221	
3222	

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